



US010418568B2

(12) **United States Patent**  
**Lam et al.**

(10) **Patent No.:** **US 10,418,568 B2**  
(45) **Date of Patent:** **Sep. 17, 2019**

(54) **ORGANIC ELECTROLUMINESCENT MATERIALS AND DEVICES**

(71) Applicant: **Universal Display Corporation**,  
Ewing, NJ (US)

(72) Inventors: **Siu Tung Lam**, Apleichau (HK);  
**Raymond Kwong**, Fo Tan (HK); **Chi Hang Lee**,  
Chaiwan (HK); **Kit Yee Tsang**, Shatin (HK)

(73) Assignee: **Universal Display Corporation**,  
Ewing, NJ (US)

(\*) Notice: Subject to any disclaimer, the term of this  
patent is extended or adjusted under 35  
U.S.C. 154(b) by 299 days.

(21) Appl. No.: **15/147,543**

(22) Filed: **May 5, 2016**

(65) **Prior Publication Data**

US 2016/0351811 A1 Dec. 1, 2016

**Related U.S. Application Data**

(60) Provisional application No. 62/169,157, filed on Jun.  
1, 2015.

(51) **Int. Cl.**  
**H01L 51/00** (2006.01)  
**C07F 5/02** (2006.01)  
(Continued)

(52) **U.S. Cl.**  
CPC ..... **H01L 51/008** (2013.01); **C07F 5/02**  
(2013.01); **C07F 5/022** (2013.01); **C07F 5/027**  
(2013.01);  
(Continued)

(58) **Field of Classification Search**  
CPC ..... H01L 51/008; H01L 51/0073; H01L  
51/0071; H01L 51/0085; H01L 51/5016;  
(Continued)

(56) **References Cited**

U.S. PATENT DOCUMENTS

3,392,181 A 7/1968 Horn  
4,769,292 A 9/1988 Tang et al.

(Continued)

FOREIGN PATENT DOCUMENTS

DE 1198372 8/1965  
EP 0650955 5/1995

(Continued)

OTHER PUBLICATIONS

Bosdet, Michael J. D. et al., "Blue Fluorescent 4a-Aza-4b-  
boraphenanthrenes", Organic Letters, 2007, vol. 9, No. 7, pp.  
1396-1398.

(Continued)

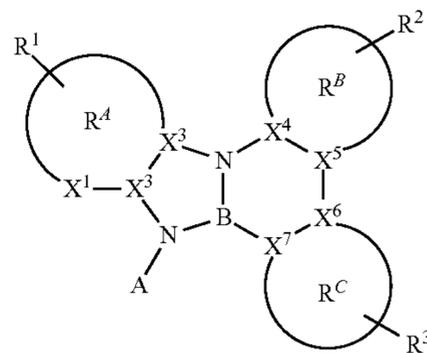
*Primary Examiner* — Jeffrey T Barton

*Assistant Examiner* — Michael Y Sun

(74) *Attorney, Agent, or Firm* — Duane Morris LLP

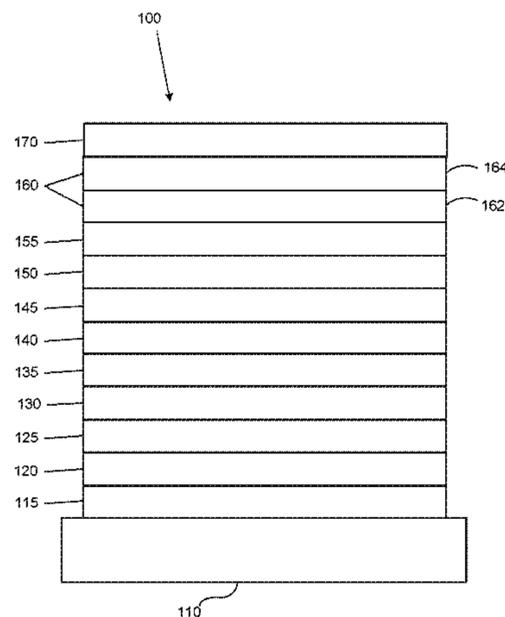
(57) **ABSTRACT**

A compound having a structure of Formula I:



Formula I

is described. In the structure of Formula I,  $R^A$ ,  $R^B$ , and  $R^C$   
are each independently 5 or 6 membered aryl or heteroaryl  
rings;  $R^1$ ,  $R^2$ ,  $R^3$ , and A are selected from a variety of  
(Continued)



substituents, including being joined or fused to form a ring; A is optionally bonded to at least one benzo or azabenzene ring to form fused rings; X<sup>1</sup> is B, C, N, O, S or Se; and X<sup>2</sup>-X<sup>7</sup> are independently B, C or N. Formulations and devices, such as an OLEDs, that include the compound containing a structure of Formula I are also described.

**20 Claims, 2 Drawing Sheets**

(51) **Int. Cl.**

**C07F 5/05** (2006.01)  
**H01L 51/50** (2006.01)  
**C09K 11/02** (2006.01)  
**C09K 11/06** (2006.01)

(52) **U.S. Cl.**

CPC ..... **C09K 11/025** (2013.01); **C09K 11/06** (2013.01); **H01L 51/0071** (2013.01); **H01L 51/0073** (2013.01); **H01L 51/0085** (2013.01); **C07F 5/05** (2013.01); **C09K 2211/1007** (2013.01); **C09K 2211/1044** (2013.01); **C09K 2211/185** (2013.01); **H01L 51/5012** (2013.01); **H01L 51/5016** (2013.01)

(58) **Field of Classification Search**

CPC ..... H01L 51/5012; C07F 5/027; C07F 5/022; C07F 5/02; C07F 5/05; C09K 11/025; C09K 11/06; C09K 2211/1044; C09K 2211/1007; C09K 2211/185

See application file for complete search history.

(56)

**References Cited**

**U.S. PATENT DOCUMENTS**

5,061,569	A	10/1991	VanSlyke et al.
5,247,190	A	9/1993	Friend et al.
5,703,436	A	12/1997	Forrest et al.
5,707,745	A	1/1998	Forrest et al.
5,834,893	A	11/1998	Bulovic et al.
5,844,363	A	12/1998	Gu et al.
6,013,982	A	1/2000	Thompson et al.
6,087,196	A	7/2000	Sturm et al.
6,091,195	A	7/2000	Forrest et al.
6,097,147	A	8/2000	Baldo et al.
6,294,398	B1	9/2001	Kim et al.
6,303,238	B1	10/2001	Thompson et al.
6,337,102	B1	1/2002	Forrest et al.
6,468,819	B1	10/2002	Kim et al.
6,528,187	B1	3/2003	Okada
6,687,266	B1	2/2004	Ma et al.
6,835,489	B2	12/2004	Kwong et al.
6,921,915	B2	7/2005	Takiguchi et al.
7,087,321	B2	8/2006	Kwong et al.
7,090,928	B2	8/2006	Thompson et al.
7,154,114	B2	12/2006	Brooks et al.
7,250,226	B2	7/2007	Tokito et al.
7,279,704	B2	10/2007	Walters et al.
7,332,232	B2	2/2008	Ma et al.
7,338,722	B2	3/2008	Thompson et al.
7,393,599	B2	7/2008	Thompson et al.
7,396,596	B2	7/2008	Takeuchi et al.
7,431,968	B1	10/2008	Shtein et al.
7,445,855	B2	11/2008	Mackenzie et al.
7,534,505	B2	5/2009	Lin et al.
2002/0034656	A1	3/2002	Thompson et al.
2002/0134984	A1	9/2002	Igarashi
2002/0158242	A1	10/2002	Son et al.
2003/0138657	A1	7/2003	Li et al.
2003/0152802	A1	8/2003	Tsuboyama et al.
2003/0162053	A1	8/2003	Marks et al.
2003/0175553	A1	9/2003	Thompson et al.

2003/0230980	A1	12/2003	Forrest et al.
2004/0036077	A1	2/2004	Ise
2004/0137267	A1	7/2004	Igarashi et al.
2004/0137268	A1	7/2004	Igarashi et al.
2004/0174116	A1	9/2004	Lu et al.
2005/0025993	A1	2/2005	Thompson et al.
2005/0112407	A1	5/2005	Ogasawara et al.
2005/0238919	A1	10/2005	Ogasawara
2005/0244673	A1	11/2005	Satoh et al.
2005/0260441	A1	11/2005	Thompson et al.
2005/0260447	A1*	11/2005	Brooks ..... C09K 11/06 428/690
2005/0260449	A1	11/2005	Walters et al.
2006/0008670	A1	1/2006	Lin et al.
2006/0202194	A1	9/2006	Jeong et al.
2006/0240279	A1	10/2006	Adamovich et al.
2006/0251923	A1	11/2006	Lin et al.
2006/0263635	A1	11/2006	Ise
2006/0280965	A1	12/2006	Kwong et al.
2007/0190359	A1	8/2007	Knowles et al.
2007/0278938	A1	12/2007	Yabunouchi et al.
2008/0015355	A1	1/2008	Schafer et al.
2008/0018221	A1	1/2008	Egen et al.
2008/0106190	A1	5/2008	Yabunouchi et al.
2008/0124572	A1	5/2008	Mizuki et al.
2008/0220265	A1	9/2008	Xia et al.
2008/0297033	A1	12/2008	Knowles et al.
2009/0008605	A1	1/2009	Kawamura et al.
2009/0009065	A1	1/2009	Nishimura et al.
2009/0017330	A1	1/2009	Iwakuma et al.
2009/0030202	A1	1/2009	Iwakuma et al.
2009/0039776	A1	2/2009	Yamada et al.
2009/0045730	A1	2/2009	Nishimura et al.
2009/0045731	A1	2/2009	Nishimura et al.
2009/0101870	A1	4/2009	Prakash et al.
2009/0108737	A1	4/2009	Kwong et al.
2009/0115316	A1	5/2009	Zheng et al.
2009/0165846	A1	7/2009	Johannes et al.
2009/0167162	A1	7/2009	Lin et al.
2009/0179554	A1	7/2009	Kuma et al.
2014/0027734	A1	1/2014	Kwong
2015/0097162	A1*	4/2015	Ono ..... H01L 51/0071 257/40

**FOREIGN PATENT DOCUMENTS**

EP	1725079	11/2006
EP	2034538	3/2009
JP	200511610	1/2005
JP	2007123392	5/2007
JP	2007254297	10/2007
JP	2008074939	4/2008
WO	01/39234	5/2001
WO	02/02714	1/2002
WO	02015654	2/2002
WO	03040257	5/2003
WO	03060956	7/2003
WO	2004093207	10/2004
WO	04107822	12/2004
WO	2005014551	2/2005
WO	2005019373	3/2005
WO	2005030900	4/2005
WO	2005089025	9/2005
WO	2005123873	12/2005
WO	2006009024	1/2006
WO	2006056418	6/2006
WO	2006072002	7/2006
WO	2006082742	8/2006
WO	2006098120	9/2006
WO	2006100298	9/2006
WO	2006103874	10/2006
WO	2006114966	11/2006
WO	2006132173	12/2006
WO	2007002683	1/2007
WO	2007004380	1/2007
WO	2007029798	A1 3/2007
WO	2007063764	6/2007
WO	2007063796	6/2007
WO	2008056746	5/2008

(56)

## References Cited

## FOREIGN PATENT DOCUMENTS

WO	2008101842	8/2008
WO	2008132085	11/2008
WO	2009000673	12/2008
WO	2009003898	1/2009
WO	2009008311	1/2009
WO	2009018009	2/2009
WO	2009021126	2/2009
WO	2009050290	4/2009
WO	2009062578	5/2009
WO	2009063833	5/2009
WO	2009066778	5/2009
WO	2009066779	5/2009
WO	2009086028	7/2009
WO	2009100991	8/2009
WO	2012121398 A1	9/2012
WO	2014042197 A1	3/2014
WO	2015053572 A1	4/2015

## OTHER PUBLICATIONS

Demott, Jessica C. et al., "Experimental and computational exploration of the dynamic behavior of (PNP)BF<sub>2</sub>, a boron compound supported by an amido/bis(phosphine) pincer ligand", *Dalton Trans.*, 2011, 40, pp. 11562-11570.

Hatakeyama, Takuji et al., "Synthesis of BN-Fused Polycyclic Aromatics via Tandem Intramolecular Electrophilic Arene Borylation", *J. Am. Chem. Soc.* 2011, 133, pps. 18614-18617.

Sachdev, Hermann et al., "Structural and Spectroscopic Properties of Aryl Substituted Aminoboranes as Model Compounds and Synthons for B/C/N Materials and New Fluorescent Systems", *Z. Anorg. Allg. Chem.* 2009, 635, pp. 2112-2119.

Taniguchi, Takuhiro et al., "TICT fluorescence of N-borylated 2,5-diarylpyrroles: a gear like dual motion in the excited state", *Dalton Trans.*, 2013, 42, pp. 620-624.

Wang, Jian et al., "Substituent Effects on Twisted Internal Charge Transfer Excited States of N-Borylated Carbazoles and (Diphenylamino)boranes", *J. Phys. Chem. A* 2012, 116, pp. 1151-1158.

K. Pilgram and F. Korte, "Über Die Umsetzung von triarylphosphiten, triarylphosphoniten und triarylboraten mit aromatischen diaminen", *Tetrahedron*, vol. 19, Issue 1, 1963, pp. 137-141 (English abstract included).

Maya, Leon, "Semiconducting Amorphous Film Containing Carbon Nitrogen and Boron", *Journal of The Electrochemical Society*, vol. 135, Issue 5, May 1988, pp. 1278-1281.

Extended European Search Report dated Jul. 22, 2016 for corresponding EP Application No. 16171317.7.

Adachi, Chihaya et al., "Organic Electroluminescent Device Having a Hole Conductor as an Emitting Layer," *Appl. Phys. Lett.*, 55(15): 1489-1491 (1989).

Adachi, Chihaya et al., "Nearly 100% Internal Phosphorescence Efficiency in an Organic Light Emitting Device," *J. Appl. Phys.*, 90(10): 5048-5051 (2001).

Adachi, Chihaya et al., "High-Efficiency Red Electrophosphorescence Devices," *Appl. Phys. Lett.* 78(11):1622-1624 (2001).

Aonuma, Masaki et al., "Material Design of Hole Transport Materials Capable of Thick-Film Formation in Organic Light Emitting Diodes," *Appl. Phys. Lett.*, Apr. 30, 2007, 90:183503-1-183503-3.

Baldo et al., "Highly Efficient Phosphorescent Emission from Organic Electroluminescent Devices," *Nature*, vol. 395, 151-154, (1998).

Baldo et al., "Very high-efficiency green organic light-emitting devices based on electrophosphorescence," *Appl. Phys. Lett.*, vol. 75, No. 1, 4-6 (1999).

Gao, Zhiqiang et al., "Bright-Blue Electroluminescence From a Silyl-Substituted ter-(phenylene-vinylene) derivative," *Appl. Phys. Lett.*, 74(6): 865-867 (1999).

Guo, Tzung-Fang et al., "Highly Efficient Electrophosphorescent Polymer Light-Emitting Devices," *Organic Electronics*, 1: 15-20 (2000).

Hamada, Yuji et al., "High Luminance in Organic Electroluminescent Devices with Bis(10-hydroxybenzo[h]quinolinato) beryllium as an Emitter," *Chem. Lett.*, 905-906 (1993).

Holmes, R.J. et al., "Blue Organic Electrophosphorescence Using Exothermic Host-Guest Energy Transfer," *Appl. Phys. Lett.*, 82(15):2422-2424 (2003).

Hu, Nan-Xing et al., "Novel High T<sub>g</sub> Hole-Transport Molecules Based on Indolo[3,2-b]carbazoles for Organic Light-Emitting Devices," *Synthetic Metals*, 111-112:421-424 (2000).

Huang, Jinsong et al., "Highly Efficient Red-Emission Polymer Phosphorescent Light-Emitting Diodes Based on Two Novel Tris(1-phenylisoquinolinato-C<sub>2</sub>,N)iridium(III) Derivatives," *Adv. Mater.*, 19:739-743 (2007).

Huang, Wei-Sheng et al., "Highly Phosphorescent Bis-Cyclometalated Iridium Complexes Containing Benzoimidazole-Based Ligands," *Chem. Mater.*, 16(12):2480-2488 (2004).

Hung, L.S. et al., "Anode Modification in Organic Light-Emitting Diodes by Low-Frequency Plasma Polymerization of CHF<sub>3</sub>," *Appl. Phys. Lett.*, 78(5):673-675 (2001).

Ikai, Masamichi et al., "Highly Efficient Phosphorescence From Organic Light-Emitting Devices with an Exciton-Block Layer," *Appl. Phys. Lett.*, 79(2):156-158 (2001).

Ikeda, Hisao et al., "P-185 Low-Drive-Voltage OLEDs with a Buffer Layer Having Molybdenum Oxide," *SID Symposium Digest*, 37:923-926 (2006).

Inada, Hiroshi and Shirota, Yasuhiko, "1,3,5-Tris[4-(diphenylamino)phenyl]benzene and its Methylsubstituted Derivatives as a Novel Class of Amorphous Molecular Materials," *J. Mater. Chem.*, 3(3):319-320 (1993).

Kanno, Hiroshi et al., "Highly Efficient and Stable Red Phosphorescent Organic Light-Emitting Device Using bis[2-(2-benzothiazoyl)phenolato]zinc(II) as host material," *Appl. Phys. Lett.*, 90:123509-1-123509-3 (2007).

Kido, Junji et al., "1,2,4-Triazole Derivative as an Electron Transport Layer in Organic Electroluminescent Devices," *Jpn. J. Appl. Phys.*, 32:L917-L920 (1993).

Kuwabara, Yoshiyuki et al., "Thermally Stable Multilayered Organic Electroluminescent Devices Using Novel Starburst Molecules, 4,4',4"-Tri(N-carbazolyl)triphenylamine (TCTA) and 4,4',4"-Tris(3-methylphenylphenyl-amino)triphenylamine (m-MTDATA), as Hole-Transport Materials," *Adv. Mater.*, 6(9):677-679 (1994).

Kwong, Raymond C. et al., "High Operational Stability of Electrophosphorescent Devices," *Appl. Phys. Lett.*, 81(1) 162-164 (2002).

Lamansky, Sergey et al., "Synthesis and Characterization of Phosphorescent Cyclometalated Iridium Complexes," *Inorg. Chem.*, 40(7):1704-1711 (2001).

Lee, Chang-Lyoul et al., "Polymer Phosphorescent Light-Emitting Devices Doped with Tris(2-phenylpyridine) Iridium as a Triplet Emitter," *Appl. Phys. Lett.*, 77(15):2280-2282 (2000).

Lo, Shih-Chun et al., "Blue Phosphorescence from Iridium(III) Complexes at Room Temperature," *Chem. Mater.*, 18(21):5119-5129 (2006).

Ma, Yuguang et al., "Triplet Luminescent Dinuclear-Gold(I) Complex-Based Light-Emitting Diodes with Low Turn-On voltage," *Appl. Phys. Lett.* 74(10):1361-1353 (1999).

Mi, Bao-Xiu et al., "Thermally Stable Hole-Transporting Material for Organic Light-Emitting Diode an Isoindole Derivative," *Chem. Mater.*, 15(16):3148-3151 (2003).

Nishida, Jun-ichi et al., "Preparation, Characterization, and Electroluminescence Characteristics of  $\alpha$ -Diimine-type Platinum(II) Complexes with Perfluorinated Phenyl Groups as Ligands," *Chem. Lett.*, 34(4): 592-593 (2005).

Niu, Yu-Hua et al., "Highly Efficient Electrophosphorescent Devices with Saturated Red Emission from a Neutral Osmium Complex," *Chem. Mater.*, 17(13):3532-3536 (2005).

Noda, Tetsuya and Shirota, Yasuhiko, "5,5'-Bis(dimesitylboryl)-2,2'-bithiophene and 5,5'-Bis(dimesitylboryl)-2,2',5',2"-terthiophene as a Novel Family of Electron-Transporting Amorphous Molecular Materials," *J. Am. Chem. Soc.*, 120 (37):9714-9716 (1998).

Okumoto, Kenji et al., "Green Fluorescent Organic Light-Emitting Device with External Quantum Efficiency of Nearly 10%," *Appl. Phys. Lett.*, 89:063504-1-063504-3 (2006).

(56)

## References Cited

## OTHER PUBLICATIONS

Palilis, Leonidas C., "High Efficiency Molecular Organic Light-Emitting Diodes Based on Silole Derivatives and Their Exciplexes," *Organic Electronics*, 4:113-121 (2003).

Paulose, Betty Marie Jennifer S. et al., "First Examples of Alkenyl Pyridines as Organic Ligands for Phosphorescent Iridium Complexes," *Adv. Mater.*, 16(22):2003-2007 (2004).

Ranjan, Sudhir et al., "Realizing Green Phosphorescent Light-Emitting Materials from Rhenium(I) Pyrazolato Diimine Complexes," *Inorg. Chem.*, 42(4):1248-1255 (2003).

Sakamoto, Youichi et al., "Synthesis, Characterization, and Electron-Transport Property of Perfluorinated Phenylene Dendrimers," *J. Am. Chem. Soc.*, 122(8):1832-1833 (2000).

Salbeck J. et al., "Low Molecular Organic Gasses for Blue Electroluminescence," *Synthetic Metals*, 91: 209-215 (1997).

Shirota, Yasuhiko et al., "Starburst Molecules Based on pi-Electron Systems as Materials for Organic Electroluminescent Devices," *Journal of Luminescence*, 72-74:985-991 (1997).

Sotoyama, Wataru et al., "Efficient Organic Light-Emitting Diodes with Phosphorescent Platinum Complexes Containing N/C/N-Coordinating Tridentate Ligand," *Appl. Phys. Lett.*, 86:153505-1-153505-3 (2005).

Sun, Yiru and Forrest, Stephen R., "High-Efficiency White Organic Light Emitting Devices with Three Separate Phosphorescent Emission Layers," *Appl. Phys. Lett.*, 91:263503-1-263503-3 (2007).

T. Ostergård et al., "Langmuir-Blodgett Light-Emitting Diodes of Poly(3-Hexylthiophene) Electro-Optical Characteristics Related to Structure," *Synthetic Metals*, 88:171-177 (1997).

Takizawa, Shin-ya et al., "Phosphorescent Iridium Complexes Based on 2-Phenylimidazo[1,2- $\alpha$ ]pyridine Ligands Tuning of Emission Color toward the Blue Region and Application to Polymer Light-Emitting Devices," *Inorg. Chem.*, 46(10):4308-4319 (2007).

Tang, C.W. and VanSlyke, S.A., "Organic Electroluminescent Diodes," *Appl. Phys. Lett.*, 51(12):913-915 (1987).

Tung, Yung-Liang et al., "Organic Light-Emitting Diodes Based on Charge-Neutral Ru II Phosphorescent Emitters," *Adv. Mater.*, 17(8):1059-1064 (2005).

Van Slyke, S. A. et al., "Organic Electroluminescent Devices with Improved Stability," *Appl. Phys. Lett.*, 69(15):2160-2162 (1996).

Wang, Y. et al., "Highly Efficient Electroluminescent Materials Based on Fluorinated Organometallic Iridium Compounds," *Appl. Phys. Lett.*, 79(4):449-451 (2001).

Wong, Keith Man-Chung et al., A Novel Class of Phosphorescent Gold(III) Alkynyl-Based Organic Light-Emitting Devices with Tunable Colour, *Chem. Commun.*, 2906-2908 (2005).

Wong, Wai-Yeung, "Multifunctional Iridium Complexes Based on Carbazole Modules as Highly Efficient Electrophosphors," *Angew. Chem. Int. Ed.*, 45:7800-7803 (2006).

\* cited by examiner

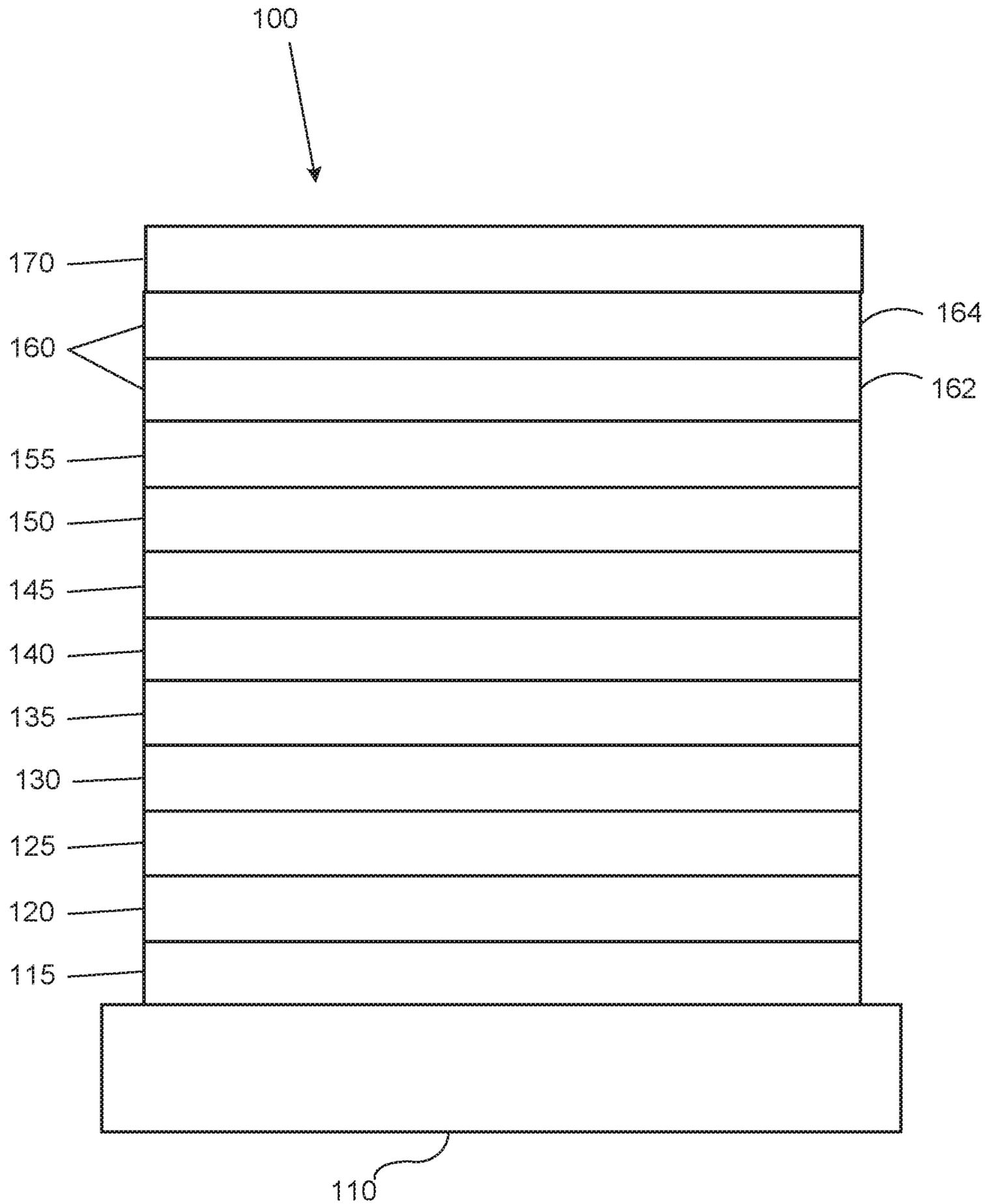


FIGURE 1

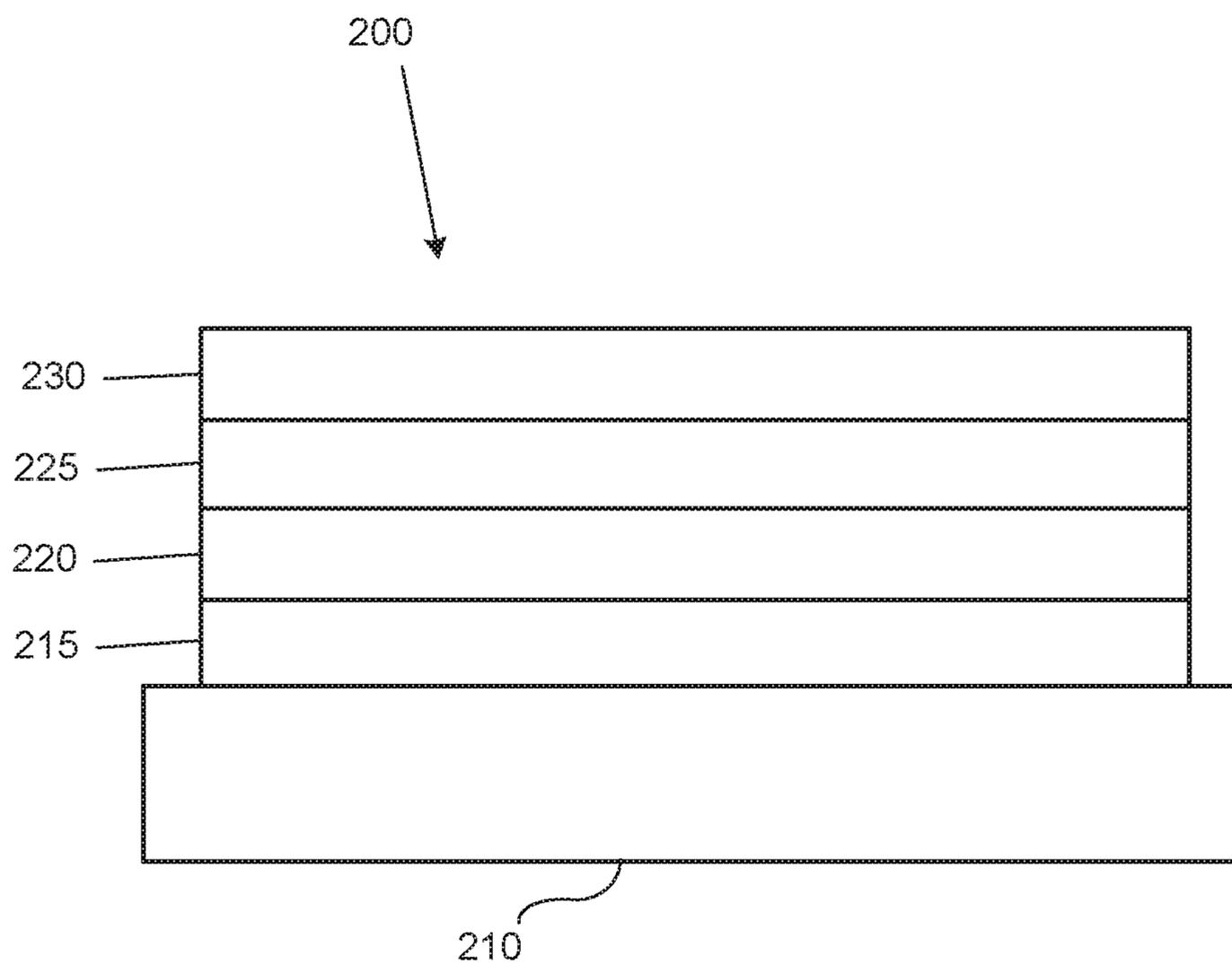


FIGURE 2

## 1

ORGANIC ELECTROLUMINESCENT  
MATERIALS AND DEVICESCROSS-REFERENCE TO RELATED  
APPLICATIONS

This application is a non-provisional of U.S. Patent Application Ser. No. 62/169,157, filed Jun. 1, 2015, the entire contents of which are incorporated herein by reference.

PARTIES TO A JOINT RESEARCH  
AGREEMENT

The claimed invention was made by, on behalf of, and/or in connection with one or more of the following parties to a joint university corporation research agreement: The Regents of the University of Michigan, Princeton University, University of Southern California, and the Universal Display Corporation. The agreement was in effect on and before the date the claimed invention was made, and the claimed invention was made as a result of activities undertaken within the scope of the agreement.

## FIELD

The present invention relates to compounds for use as electroluminescent materials, such as hosts, and devices, such as organic light emitting diodes, including the same.

## BACKGROUND

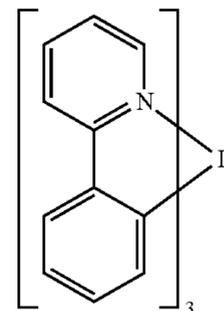
Opto-electronic devices that make use of organic materials are becoming increasingly desirable for a number of reasons. Many of the materials used to make such devices are relatively inexpensive, so organic opto-electronic devices have the potential for cost advantages over inorganic devices. In addition, the inherent properties of organic materials, such as their flexibility, may make them well suited for particular applications such as fabrication on a flexible substrate. Examples of organic opto-electronic devices include organic light emitting diodes/devices (OLEDs), organic phototransistors, organic photovoltaic cells, and organic photodetectors. For OLEDs, the organic materials may have performance advantages over conventional materials. For example, the wavelength at which an organic emissive layer emits light may generally be readily tuned with appropriate dopants.

OLEDs make use of thin organic films that emit light when voltage is applied across the device. OLEDs are becoming an increasingly interesting technology for use in applications such as flat panel displays, illumination, and backlighting. Several OLED materials and configurations are described in U.S. Pat. Nos. 5,844,363, 6,303,238, and 5,707,745, which are incorporated herein by reference in their entirety.

One application for phosphorescent emissive molecules is a full color display. Industry standards for such a display call for pixels adapted to emit particular colors, referred to as "saturated" colors. In particular, these standards call for saturated red, green, and blue pixels. Alternatively the OLED can be designed to emit white light. In conventional liquid crystal displays emission from a white backlight is filtered using absorption filters to produce red, green and blue emission. The same technique can also be used with OLEDs. The white OLED can be either a single EML device or a stack structure. Color may be measured using CIE coordinates, which are well known to the art.

## 2

One example of a green emissive molecule is tris(2-phenylpyridine) iridium, denoted Ir(ppy)<sub>3</sub>, which has the following structure:



In this, and later figures herein, we depict the dative bond from nitrogen to metal (here, Ir) as a straight line.

As used herein, the term "organic" includes polymeric materials as well as small molecule organic materials that may be used to fabricate organic opto-electronic devices. "Small molecule" refers to any organic material that is not a polymer, and "small molecules" may actually be quite large. Small molecules may include repeat units in some circumstances. For example, using a long chain alkyl group as a substituent does not remove a molecule from the "small molecule" class. Small molecules may also be incorporated into polymers, for example as a pendent group on a polymer backbone or as a part of the backbone. Small molecules may also serve as the core moiety of a dendrimer, which consists of a series of chemical shells built on the core moiety. The core moiety of a dendrimer may be a fluorescent or phosphorescent small molecule emitter. A dendrimer may be a "small molecule." and it is believed that all dendrimers currently used in the field of OLEDs are small molecules.

As used herein, "top" means furthest away from the substrate, while "bottom" means closest to the substrate. Where a first layer is described as "disposed over" a second layer, the first layer is disposed further away from substrate. There may be other layers between the first and second layer, unless it is specified that the first layer is "in contact with" the second layer. For example, a cathode may be described as "disposed over" an anode, even though there are various organic layers in between.

As used herein, "solution processable" means capable of being dissolved, dispersed, or transported in and/or deposited from a liquid medium, either in solution or suspension form.

A ligand may be referred to as "photoactive" when it is believed that the ligand directly contributes to the photoactive properties of an emissive material. A ligand may be referred to as "ancillary" when it is believed that the ligand does not contribute to the photoactive properties of an emissive material, although an ancillary ligand may alter the properties of a photoactive ligand.

As used herein, and as would be generally understood by one skilled in the art, a first "Highest Occupied Molecular Orbital" (HOMO) or "Lowest Unoccupied Molecular Orbital" (LUMO) energy level is "greater than" or "higher than" a second HOMO or LUMO energy level if the first energy level is closer to the vacuum energy level. Since ionization potentials (IP) are measured as a negative energy relative to a vacuum level, a higher HOMO energy level corresponds to an IP having a smaller absolute value (an IP that is less negative). Similarly, a higher LUMO energy level corresponds to an electron affinity (EA) having a smaller absolute value (an EA that is less negative). On a conven-

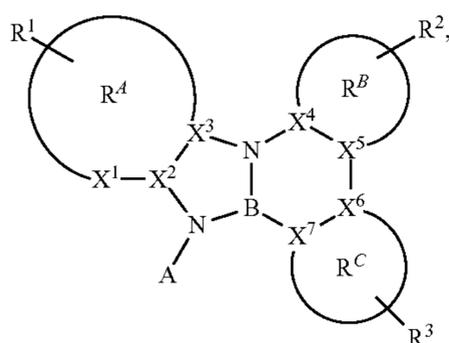
tional energy level diagram, with the vacuum level at the top, the LUMO energy level of a material is higher than the HOMO energy level of the same material. A “higher” HOMO or LUMO energy level appears closer to the top of such a diagram than a “lower” HOMO or LUMO energy level.

As used herein, and as would be generally understood by one skilled in the art, a first work function is “greater than” or “higher than” a second work function if the first work function has a higher absolute value. Because work functions are generally measured as negative numbers relative to vacuum level, this means that a “higher” work function is more negative. On a conventional energy level diagram, with the vacuum level at the top, a “higher” work function is illustrated as further away from the vacuum level in the downward direction. Thus, the definitions of HOMO and LUMO energy levels follow a different convention than work functions.

More details on OLEDs, and the definitions described above, can be found in U.S. Pat. No. 7,279,704, which is incorporated herein by reference in its entirety.

### SUMMARY

According to an embodiment, a compound is provided that has the structure of Formula I:



is described.

In the structure of Formula I:

$R^A$ ,  $R^B$ , and  $R^C$  are each independently 5 or 6 membered aryl or heteroaryl rings;

$R^1$ ,  $R^2$ , and  $R^3$  each independently represent no substitutions or up to the maximum available substitutions;

$R^1$ ,  $R^2$ , and  $R^3$  are each independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphine, a substituent of Formula I, and combinations thereof;

any adjacent  $R^1$ ,  $R^2$ , and  $R^3$  are optionally joined or fused to form a ring;

A is selected from the group consisting of hydrogen, deuterium halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphine, a substituent of Formula I, and combinations thereof;

A is optionally bonded to at least one benzo or azabenzene ring to form fused rings;

$X^1$  is B, C, N, O, S or Se; and

$X^2$ - $X^7$  are independently B, C or N.

According to another embodiment, an organic light emitting diode/device (OLED) is also provided. The OLED can include an anode, a cathode, and an organic layer, disposed between the anode and the cathode. The organic layer can include a compound comprising a structure of Formula I. According to yet another embodiment, the organic light emitting device is incorporated into a device selected from a consumer product, an electronic component module, and/or a lighting panel.

According to yet another embodiment, a formulation containing a compound comprising a structure of Formula I is provided.

### BRIEF DESCRIPTION OF THE DRAWINGS

FIG. 1 shows an organic light emitting device.

FIG. 2 shows an inverted organic light emitting device that does not have a separate electron transport layer.

### DETAILED DESCRIPTION

Generally, an OLED comprises at least one organic layer disposed between and electrically connected to an anode and a cathode. When a current is applied, the anode injects holes and the cathode injects electrons into the organic layer(s). The injected holes and electrons each migrate toward the oppositely charged electrode. When an electron and hole localize on the same molecule, an “exciton,” which is a localized electron-hole pair having an excited energy state, is formed. Light is emitted when the exciton relaxes via a photoemissive mechanism. In some cases, the exciton may be localized on an excimer or an exciplex. Non-radiative mechanisms, such as thermal relaxation, may also occur, but are generally considered undesirable.

The initial OLEDs used emissive molecules that emitted light from their singlet states (“fluorescence”) as disclosed, for example, in U.S. Pat. No. 4,769,292, which is incorporated by reference in its entirety. Fluorescent emission generally occurs in a time frame of less than 10 nanoseconds.

More recently, OLEDs having emissive materials that emit light from triplet states (“phosphorescence”) have been demonstrated. Baldo et al., “Highly Efficient Phosphorescent Emission from Organic Electroluminescent Devices,” *Nature*, vol. 395, 151-154, 1998; (“Baldo-I”) and Baldo et al., “Very high-efficiency green organic light-emitting devices based on electrophosphorescence,” *Appl. Phys. Lett.*, vol. 75, No. 3, 4-6 (1999) (“Baldo-II”), are incorporated by reference in their entireties. Phosphorescence is described in more detail in U.S. Pat. No. 7,279,704 at cols. 5-6, which are incorporated by reference.

FIG. 1 shows an organic light emitting device 100. The figures are not necessarily drawn to scale. Device 100 may include a substrate 110, an anode 115, a hole injection layer 120, a hole transport layer 125, an electron blocking layer 130, an emissive layer 135, a hole blocking layer 140, an electron transport layer 145, an electron injection layer 150, a protective layer 155, a cathode 160, and a barrier layer 170. Cathode 160 is a compound cathode having a first conductive layer 162 and a second conductive layer 164. Device 100 may be fabricated by depositing the layers described, in order. The properties and functions of these various layers, as well as example materials, are described in more detail in U.S. Pat. No. 7,279,704 at cols. 6-10, which are incorporated by reference.

More examples for each of these layers are available. For example, a flexible and transparent substrate-anode combi-

nation is disclosed in U.S. Pat. No. 5,844,363, which is incorporated by reference in its entirety. An example of a p-doped hole transport layer is m-MTDATA doped with F<sub>4</sub>-TCNQ at a molar ratio of 50:1, as disclosed in U.S. Patent Application Publication No. 2003/0230980, which is incorporated by reference in its entirety. Examples of emissive and host materials are disclosed in U.S. Pat. No. 6,303,238 to Thompson et al., which is incorporated by reference in its entirety. An example of an n-doped electron transport layer is BPhen doped with Li at a molar ratio of 1:1, as disclosed in U.S. Patent Application Publication No. 2003/0230980, which is incorporated by reference in its entirety. U.S. Pat. Nos. 5,703,436 and 5,707,745, which are incorporated by reference in their entireties, disclose examples of cathodes including compound cathodes having a thin layer of metal such as Mg:Ag with an overlying transparent, electrically-conductive, sputter-deposited ITO layer. The theory and use of blocking layers is described in more detail in U.S. Pat. No. 6,097,147 and U.S. Patent Application Publication No. 2003/0230980, which are incorporated by reference in their entireties. Examples of injection layers are provided in U.S. Patent Application Publication No. 2004/0174116, which is incorporated by reference in its entirety. A description of protective layers may be found in U.S. Patent Application Publication No. 2004/0174116, which is incorporated by reference in its entirety.

FIG. 2 shows an inverted OLED **200**. The device includes a substrate **210**, a cathode **215**, an emissive layer **220**, a hole transport layer **225**, and an anode **230**. Device **200** may be fabricated by depositing the layers described, in order. Because the most common OLED configuration has a cathode disposed over the anode, and device **200** has cathode **215** disposed under anode **230**, device **200** may be referred to as an “inverted” OLED. Materials similar to those described with respect to device **100** may be used in the corresponding layers of device **200**. FIG. 2 provides one example of how some layers may be omitted from the structure of device **100**.

The simple layered structure illustrated in FIGS. 1 and 2 is provided by way of non-limiting example, and it is understood that embodiments of the invention may be used in connection with a wide variety of other structures. The specific materials and structures described are exemplary in nature, and other materials and structures may be used. Functional OLEDs may be achieved by combining the various layers described in different ways, or layers may be omitted entirely, based on design, performance, and cost factors. Other layers not specifically described may also be included. Materials other than those specifically described may be used. Although many of the examples provided herein describe various layers as comprising a single material, it is understood that combinations of materials, such as a mixture of host and dopant, or more generally a mixture, may be used. Also, the layers may have various sublayers. The names given to the various layers herein are not intended to be strictly limiting. For example, in device **200**, hole transport layer **225** transports holes and injects holes into emissive layer **220**, and may be described as a hole transport layer or a hole injection layer. In one embodiment, an OLED may be described as having an “organic layer” disposed between a cathode and an anode. This organic layer may comprise a single layer, or may further comprise multiple layers of different organic materials as described, for example, with respect to FIGS. 1 and 2.

Structures and materials not specifically described may also be used, such as OLEDs comprised of polymeric materials (PLEDs) such as disclosed in U.S. Pat. No. 5,247,

190 to Friend et al., which is incorporated by reference in its entirety. By way of further example, OLEDs having a single organic layer may be used. OLEDs may be stacked, for example as described in U.S. Pat. No. 5,707,745 to Forrest et al, which is incorporated by reference in its entirety. The OLED structure may deviate from the simple layered structure illustrated in FIGS. 1 and 2. For example, the substrate may include an angled reflective surface to improve out-coupling, such as a mesa structure as described in U.S. Pat. No. 6,091,195 to Forrest et al., and/or a pit structure as described in U.S. Pat. No. 5,834,893 to Bulovic et al., which are incorporated by reference in their entireties.

Unless otherwise specified, any of the layers of the various embodiments may be deposited by any suitable method. For the organic layers, preferred methods include thermal evaporation, ink-jet, such as described in U.S. Pat. Nos. 6,013,982 and 6,087,196, which are incorporated by reference in their entireties, organic vapor phase deposition (OVPD), such as described in U.S. Pat. No. 6,337,102 to Forrest et al., which is incorporated by reference in its entirety, and deposition by organic vapor jet printing (OVJP), such as described in U.S. Pat. No. 7,431,968, which is incorporated by reference in its entirety. Other suitable deposition methods include spin coating and other solution based processes. Solution based processes are preferably carried out in nitrogen or an inert atmosphere. For the other layers, preferred methods include thermal evaporation. Preferred patterning methods include deposition through a mask, cold welding such as described in U.S. Pat. Nos. 6,294,398 and 6,468,819, which are incorporated by reference in their entireties, and patterning associated with some of the deposition methods such as ink-jet and OVJD. Other methods may also be used. The materials to be deposited may be modified to make them compatible with a particular deposition method. For example, substituents such as alkyl and aryl groups, branched or unbranched, and preferably containing at least 3 carbons, may be used in small molecules to enhance their ability to undergo solution processing. Substituents having 20 carbons or more may be used, and 3-20 carbons is a preferred range. Materials with asymmetric structures may have better solution processability than those having symmetric structures, because asymmetric materials may have a lower tendency to recrystallize. Dendrimer substituents may be used to enhance the ability of small molecules to undergo solution processing.

Devices fabricated in accordance with embodiments of the present invention may further optionally comprise a barrier layer. One purpose of the barrier layer is to protect the electrodes and organic layers from damaging exposure to harmful species in the environment including moisture, vapor and/or gases, etc. The barrier layer may be deposited over, under or next to a substrate, an electrode, or over any other parts of a device including an edge. The barrier layer may comprise a single layer, or multiple layers. The barrier layer may be formed by various known chemical vapor deposition techniques and may include compositions having a single phase as well as compositions having multiple phases. Any suitable material or combination of materials may be used for the barrier layer. The barrier layer may incorporate an inorganic or an organic compound or both. The preferred barrier layer comprises a mixture of a polymeric material and a non-polymeric material as described in U.S. Pat. No. 7,968,146, PCT Pat. Application Nos. PCT/US2007/023098 and PCT/US2009/042829, which are herein incorporated by reference in their entireties. To be considered a “mixture”, the aforesaid polymeric and non-polymeric materials comprising the barrier layer should be

deposited under the same reaction conditions and/or at the same time. The weight ratio of polymeric to non-polymeric material may be in the range of 95:5 to 5:95. The polymeric material and the non-polymeric material may be created from the same precursor material. In one example, the mixture of a polymeric material and a non-polymeric material consists essentially of polymeric silicon and inorganic silicon.

Devices fabricated in accordance with embodiments of the invention can be incorporated into a wide variety of electronic component modules (or units) that can be incorporated into a variety of electronic products or intermediate components. Examples of such electronic products or intermediate components include display screens, lighting devices such as discrete light source devices or lighting panels, etc. that can be utilized by the end-user product manufacturers. Such electronic component modules can optionally include the driving electronics and/or power source(s). Devices fabricated in accordance with embodiments of the invention can be incorporated into a wide variety of consumer products that have one or more of the electronic component modules (or units) incorporated therein. Such consumer products would include any kind of products that include one or more light source(s) and/or one or more of some type of visual displays. Some examples of such consumer products include flat panel displays, computer monitors, medical monitors, televisions, billboards, lights for interior or exterior illumination and/or signaling, heads-up displays, fully or partially transparent displays, flexible displays, laser printers, telephones, cell phones, tablets, phablets, personal digital assistants (PDAs), wearable device, laptop computers, digital cameras, camcorders, viewfinders, micro-displays, 3-D displays, vehicles, a large area wall, theater or stadium screen, or a sign. Various control mechanisms may be used to control devices fabricated in accordance with the present invention, including passive matrix and active matrix. Many of the devices are intended for use in a temperature range comfortable to humans, such as 18 degrees C. to 30 degrees C., and more preferably at room temperature (20-25 degrees C.), but could be used outside this temperature range, for example, from -40 degree C. to +80 degree C.

The materials and structures described herein may have applications in devices other than OLEDs. For example, other optoelectronic devices such as organic solar cells and organic photodetectors may employ the materials and structures. More generally, organic devices, such as organic transistors, may employ the materials and structures.

The term "halo," "halogen," or "halide" as used herein includes fluorine, chlorine, bromine, and iodine.

The term "alkyl" as used herein contemplates both straight and branched chain alkyl radicals. Preferred alkyl groups are those containing from one to fifteen carbon atoms and includes methyl, ethyl, propyl, 1-methylethyl, butyl, 1-methylpropyl, 2-methylpropyl, pentyl, 1-methylbutyl, 2-methylbutyl, 3-methylbutyl, 1,1-dimethylpropyl, 1,2-dimethylpropyl, 2,2-dimethylpropyl, and the like. Additionally, the alkyl group may be optionally substituted.

The term "cycloalkyl" as used herein contemplates cyclic alkyl radicals. Preferred cycloalkyl groups are those containing 3 to 10 ring carbon atoms and includes cyclopropyl, cyclopentyl, cyclohexyl, adamantyl, and the like. Additionally, the cycloalkyl group may be optionally substituted.

The term "alkenyl" as used herein contemplates both straight and branched chain alkene radicals. Preferred alk-

enyl groups are those containing two to fifteen carbon atoms. Additionally, the alkenyl group may be optionally substituted.

The term "alkynyl" as used herein contemplates both straight and branched chain alkyne radicals. Preferred alkynyl groups are those containing two to fifteen carbon atoms. Additionally, the alkynyl group may be optionally substituted.

The terms "aralkyl" or "arylalkyl" as used herein are used interchangeably and contemplate an alkyl group that has as a substituent an aromatic group. Additionally, the aralkyl group may be optionally substituted.

The term "heterocyclic group" as used herein contemplates aromatic and non-aromatic cyclic radicals. Heteroaromatic cyclic radicals also means heteroaryl. Preferred hetero-non-aromatic cyclic groups are those containing 3 to 7 ring atoms which includes at least one hetero atom, and includes cyclic amines such as morpholino, piperdino, pyrrolidino, and the like, and cyclic ethers, such as tetrahydrofuran, tetrahydropyran, and the like. Additionally, the heterocyclic group may be optionally substituted.

The term "aryl" or "aromatic group" as used herein contemplates single-ring groups and polycyclic ring systems. The polycyclic rings may have two or more rings in which two carbons are common to two adjoining rings (the rings are "fused") wherein at least one of the rings is aromatic. e.g., the other rings can be cycloalkyls, cycloalkenyls, aryl, heterocycles, and/or heteroaryls. Preferred aryl groups are those containing six to thirty carbon atoms, preferably six to twenty carbon atoms, more preferably six to twelve carbon atoms. Especially preferred is an aryl group having six carbons, ten carbons or twelve carbons. Suitable aryl groups include phenyl, biphenyl, triphenyl, triphenylene, tetraphenylene, naphthalene, anthracene, phenalene, phenanthrene, fluorene, pyrene, chrysene, perylene, and azulene, preferably phenyl, biphenyl, triphenyl, triphenylene, fluorene, and naphthalene. Additionally, the aryl group may be optionally substituted.

The term "heteroaryl" as used herein contemplates single-ring hetero-aromatic groups that may include from one to five heteroatoms. The term heteroaryl also includes polycyclic hetero-aromatic systems having two or more rings in which two atoms are common to two adjoining rings (the rings are "fused") wherein at least one of the rings is a heteroaryl, e.g., the other rings can be cycloalkyls, cycloalkenyls, aryl, heterocycles, and/or heteroaryls. Preferred heteroaryl groups are those containing three to thirty carbon atoms, preferably three to twenty carbon atoms, more preferably three to twelve carbon atoms. Suitable heteroaryl groups include dibenzothiophene, dibenzofuran, dibenzoselenophene, furan, thiophene, benzofuran, benzothiophene, benzoselenophene, carbazole, indolocarbazole, pyridylindole, pyrrolodipyridine, pyrazole, imidazole, triazole, oxazole, thiazole, oxadiazole, oxatriazole, dioxazole, thiadiazole, pyridine, pyridazine, pyrimidine, pyrazine, triazine, oxazine, oxathiazine, oxadiazine, indole, benzimidazole, indazole, indoxazine, benzoxazole, benzisoxazole, benzothiazole, quinoline, isoquinoline, cinnoline, quinazoline, quinoxaline, naphthyridine, phthalazine, pteridine, xanthene, acridine, phenazine, phenothiazine, phenoxazine, benzofuropyridine, furodipyridine, benzothienopyridine, thienodipyridine, benzoselenophenopyridine, and selenophenodipyridine, preferably dibenzothiophene, dibenzofuran, dibenzoselenophene, carbazole, indolocarbazole, imidazole, pyridine, triazine, benzimidazole, 1,2-azaborine,

1,3-azaborine, 1,4-azaborine, borazine, and aza-analogs thereof. Additionally, the heteroaryl group may be optionally substituted.

The alkyl, cycloalkyl, alkenyl, alkynyl, aralkyl, heterocyclic group, aryl, and heteroaryl may be optionally substituted with one or more substituents selected from the group consisting of hydrogen, deuterium, halogen, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, cyclic amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acid, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof.

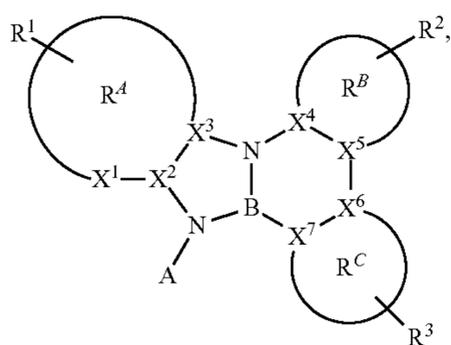
As used herein, "substituted" indicates that a substituent other than H is bonded to the relevant position, such as carbon. Thus, for example, where  $R^1$  is mono-substituted, then one  $R^1$  must be other than H. Similarly, where  $R^1$  is di-substituted, then two of  $R^1$  must be other than H. Similarly, where  $R^1$  is unsubstituted,  $R^1$  is hydrogen for all available positions.

The "aza" designation in the fragments described herein, i.e. aza-dibenzofuran, aza-dibenzothiophene, etc. means that one or more of the C—H groups in the respective fragment can be replaced by a nitrogen atom, for example, and without any limitation, azatriphenylene encompasses both dibenzo[f,h]quinoxaline and dibenzo[f,h]quinoline. One of ordinary skill in the art can readily envision other nitrogen analogs of the aza-derivatives described above, and all such analogs are intended to be encompassed by the terms as set forth herein.

It is to be understood that when a molecular fragment is described as being a substituent or otherwise attached to another moiety, its name may be written as if it were a fragment (e.g. phenyl, phenylene, naphthyl, dibenzofuryl) or as if it were the whole molecule (e.g. benzene, naphthalene, dibenzofuran). As used herein, these different ways of designating a substituent or attached fragment are considered to be equivalent.

High triplet hosts are important to providing good device efficiency for blue and green phosphorescent OLEDs. Azaborine containing hosts may be beneficial since the B—N linkage may increase the triplet energy without losing the aromatic character which is important to stabilization of charge.

According to one embodiment, a compound having a structure of Formula I:



is described.

In the structure of Formula I:

$R^A$ ,  $R^B$ , and  $R^C$  are each independently 5 or 6 membered aryl or heteroaryl rings;

$R^1$ ,  $R^2$ , and  $R^3$  each independently represent no substitutions or up to the maximum available substitutions:

$R^1$ ,  $R^2$ , and  $R^3$  are each independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphine, a substituent of Formula I, and combinations thereof:

wherein any adjacent  $R^1$ ,  $R^2$ , and  $R^3$  are optionally joined or fused to form a ring;

A is selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphine, a substituent of Formula I, and combinations thereof;

A is optionally bonded to at least one benzo or azabenzene ring to form fused rings;

$X^1$  is B, C, N, O, S or Se; and

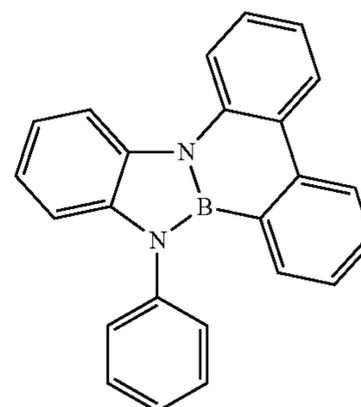
$X^2$ - $X^7$  are independently B, C or N.

In some embodiments, the compound is a dimer. In some embodiments, any  $R^1$ ,  $R^2$ , and  $R^3$  substituents are optionally joined or fused to form a 5- or 6-membered ring, which may be further substituted based on the definition of  $R^1$ ,  $R^2$ , and  $R^3$ .

In some embodiments,  $X^1$ - $X^6$  are C, and  $X^7$  is C or N.

In some embodiments, A is aryl or heteroaryl. In some embodiments, A is selected from the group consisting of phenyl, carbazole, azacarbazole, dibenzofuran, dibenzothiophene, dibenzoselenophene, azadibenzofuran, azadibenzothiophene, azadibenzoselenophene, triphenylene, azatriphenylene, and combinations thereof, and A is optionally further substituted by one or more substituent B. In such embodiments, B is selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphine, and combinations thereof; and B is optionally bonded to at least one benzo or azabenzene ring to form a fused ring.

In some embodiments, the compound is selected from the group consisting of:

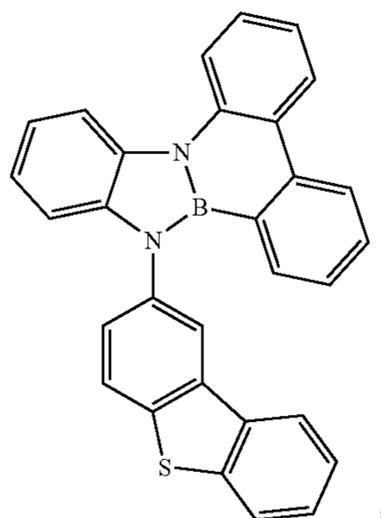
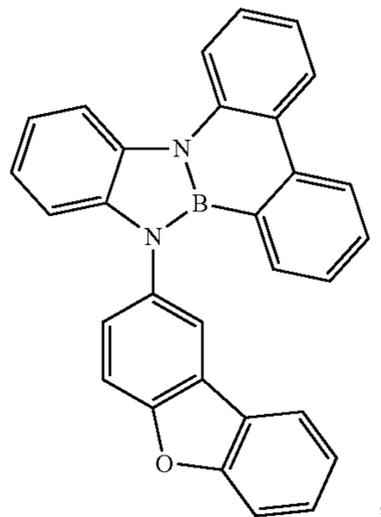
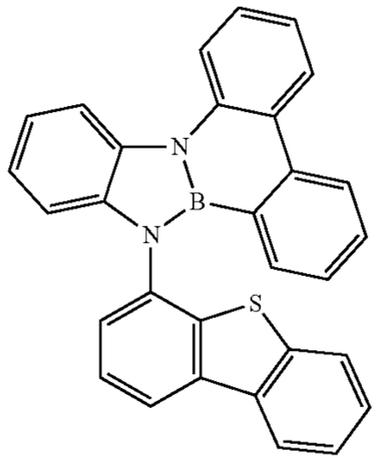
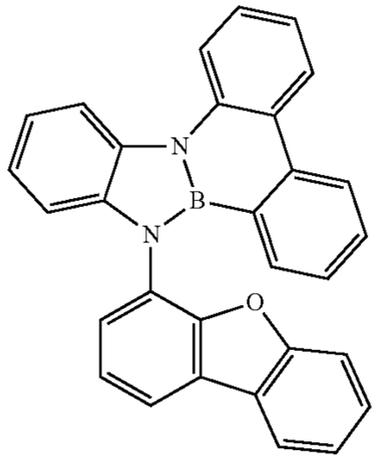


Compound 34

Formula I

**11**

-continued

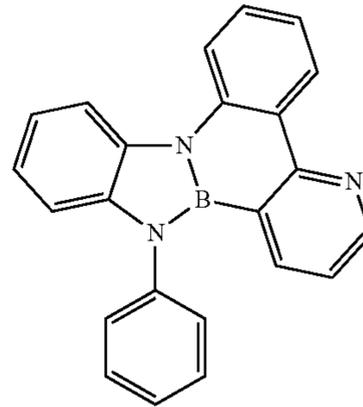


**12**

-continued

Compound 35

5

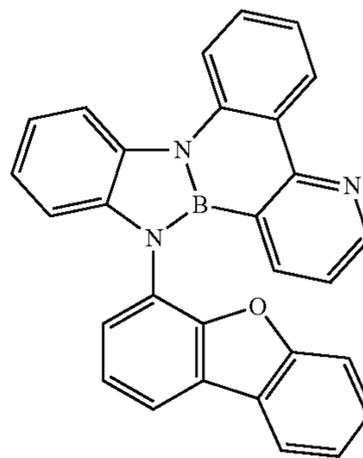


10

15

Compound 36

20

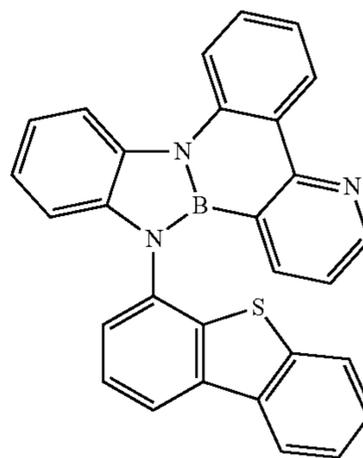


25

30

Compound 37

35



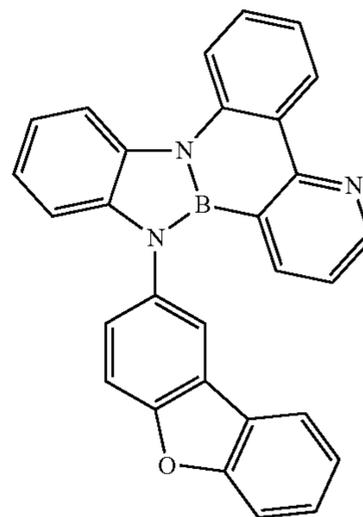
40

45

50

Compound 38

55



60

65

Compound 39

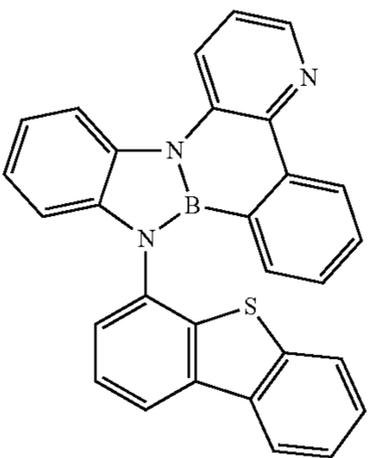
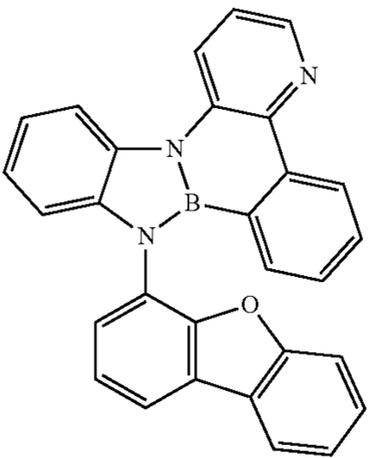
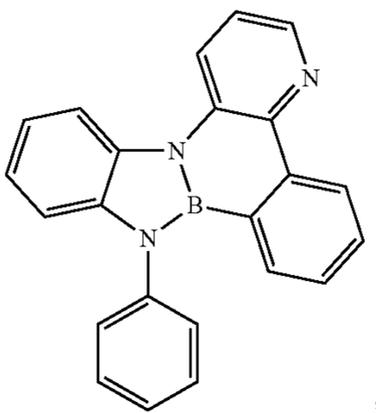
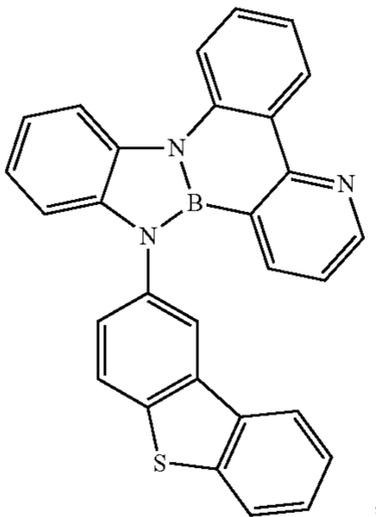
Compound 40

Compound 41

Compound 42

**13**

-continued



**14**

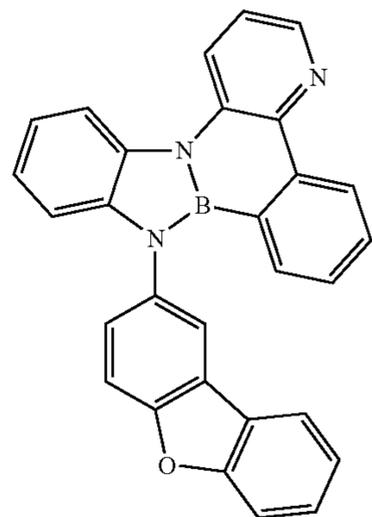
-continued

Compound 43

5

10

15

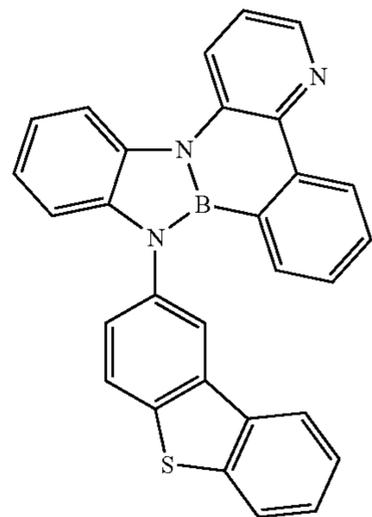


Compound 44

20

25

30



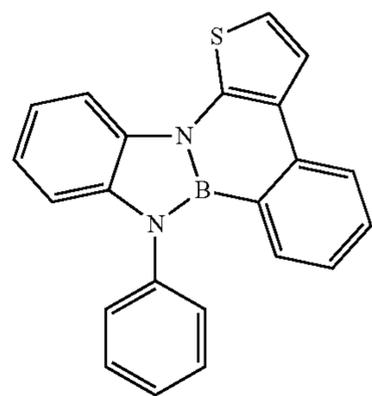
Compound 45

35

40

45

50

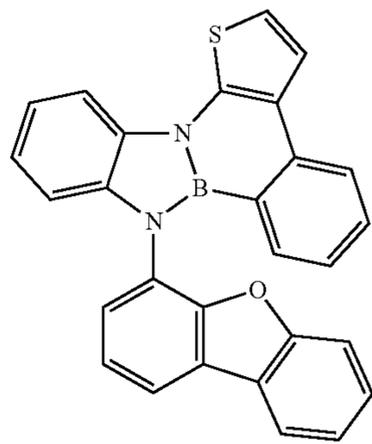


Compound 46

55

60

65



Compound 47

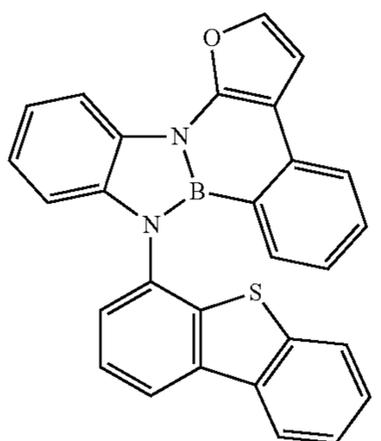
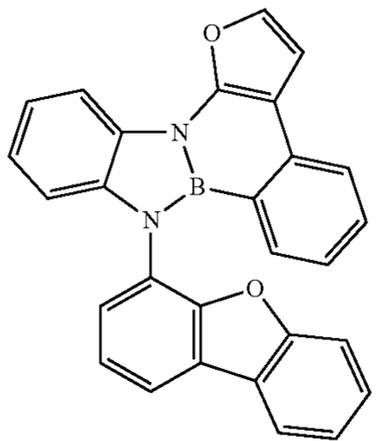
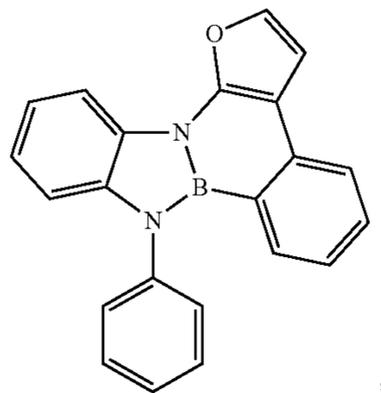
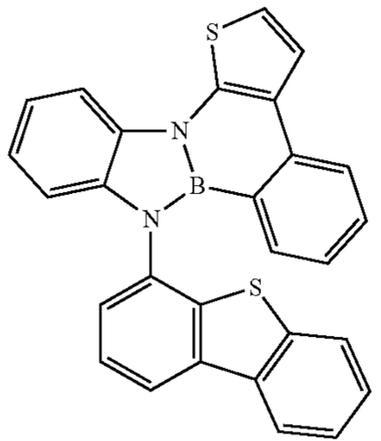
Compound 48

Compound 79

Compound 80

**15**

-continued



**16**

-continued

Compound 81

5

10

15

Compound 82

20

25

30

Compound 83

40

45

50

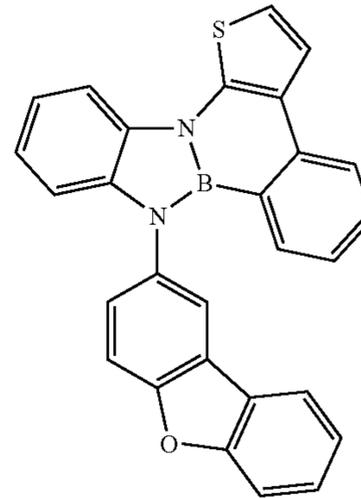
Compound 84

55

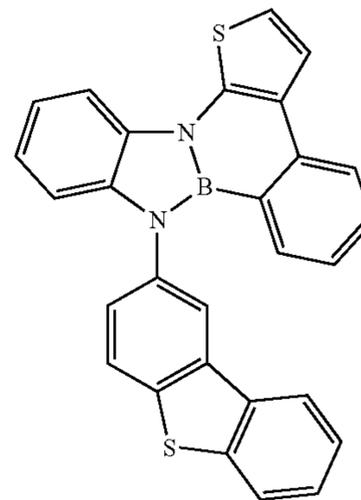
60

65

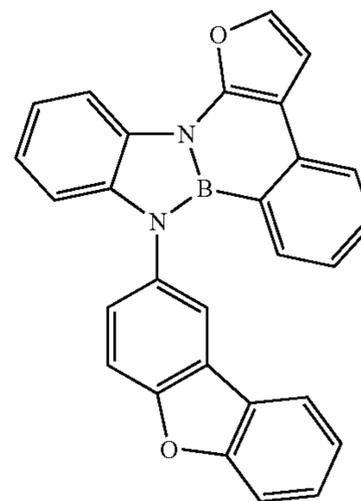
Compound 85



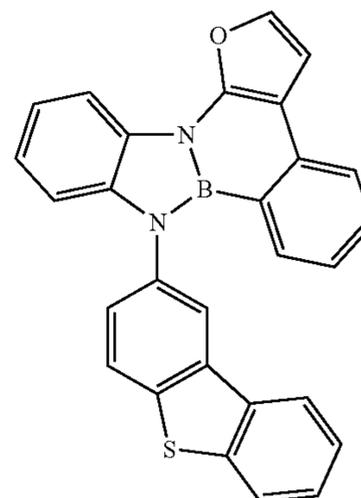
Compound 86



Compound 87

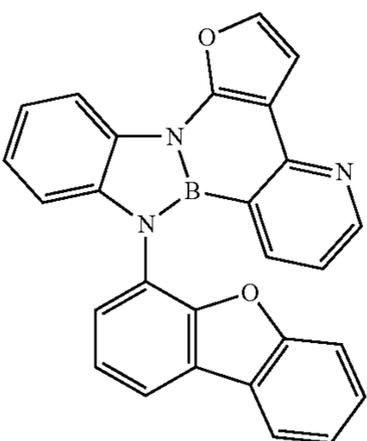
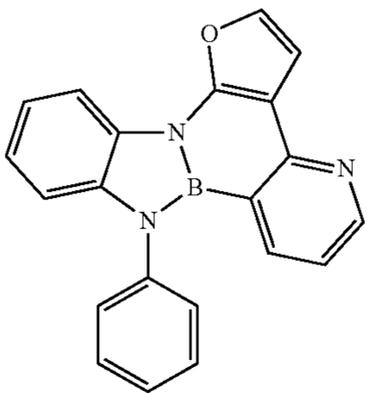
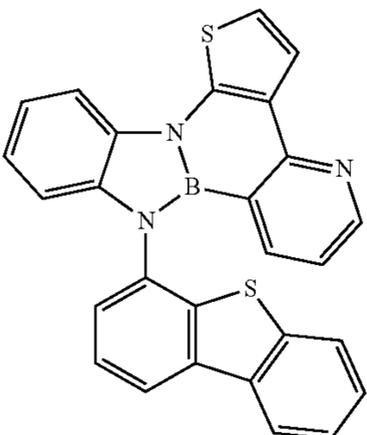
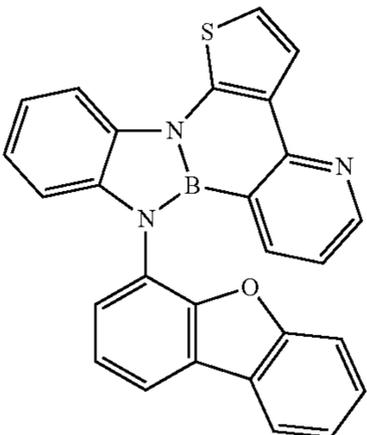
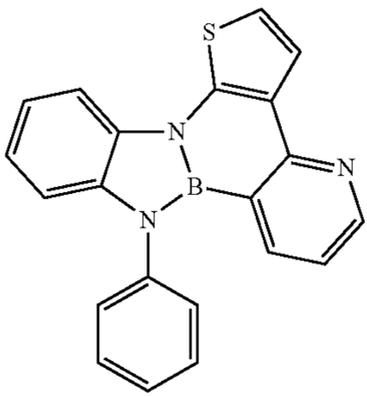


Compound 88



**17**

-continued

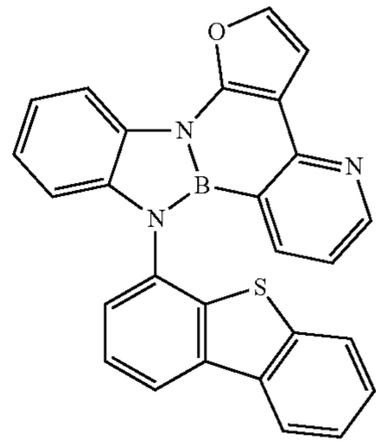


**18**

-continued

Compound 89

5



Compound 90

15

Compound 91

30

Compound 92

45

Compound 93

55

60

65

Compound 94

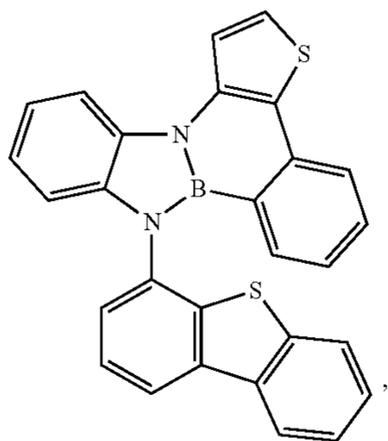
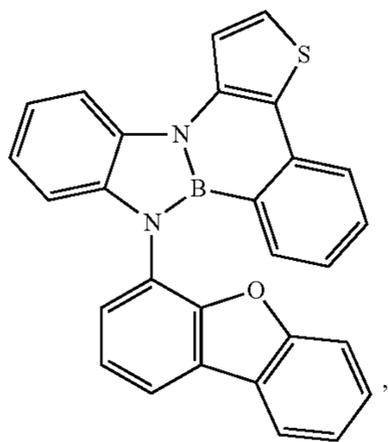
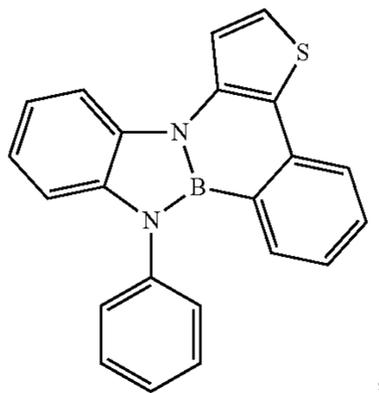
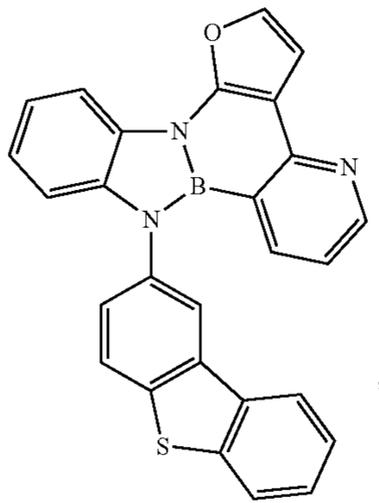
Compound 95

Compound 96

Compound 97

19

-continued



20

-continued

Compound 98

5

10

15

Compound 99

20

25

30

Compound 100

35

40

45

50

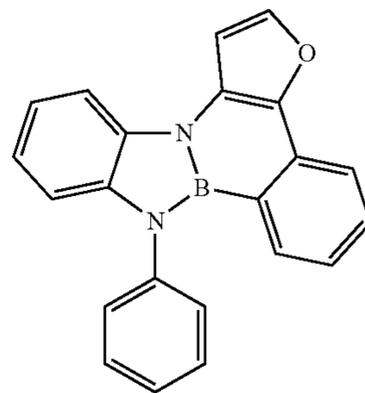
Compound 101

55

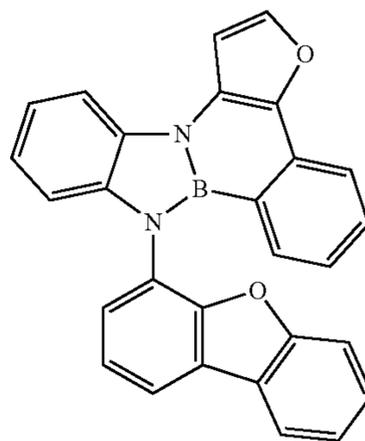
60

65

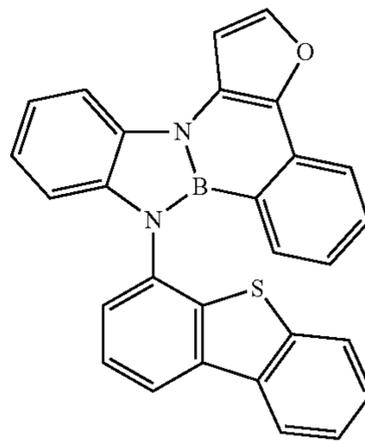
Compound 102



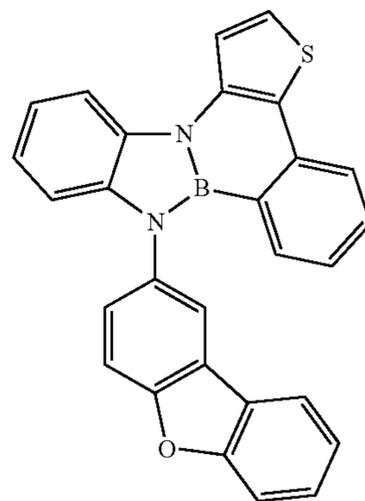
Compound 103



Compound 104

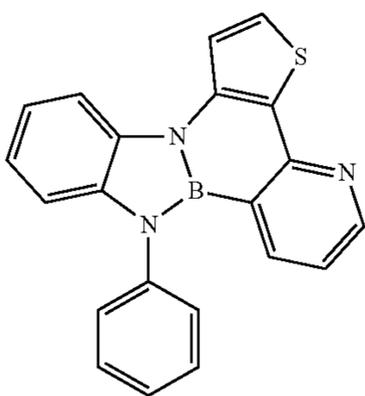
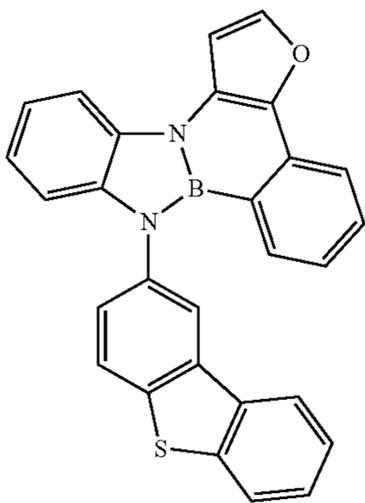
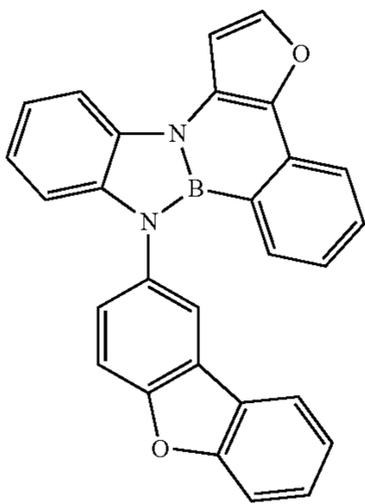
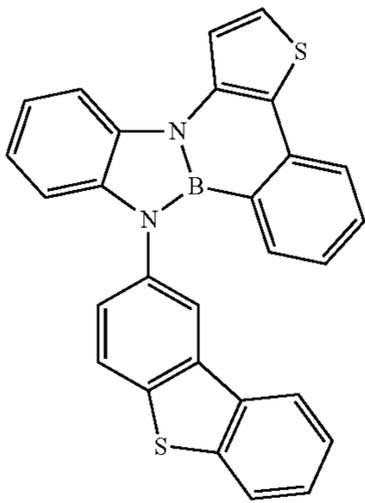


Compound 105



**21**

-continued

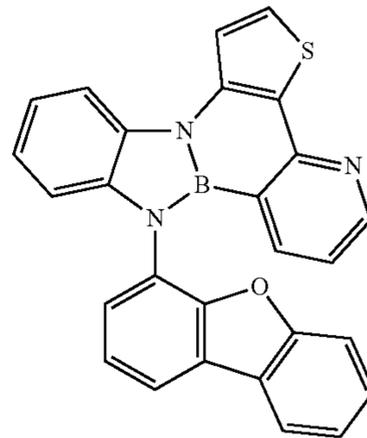


**22**

-continued

Compound 106

5

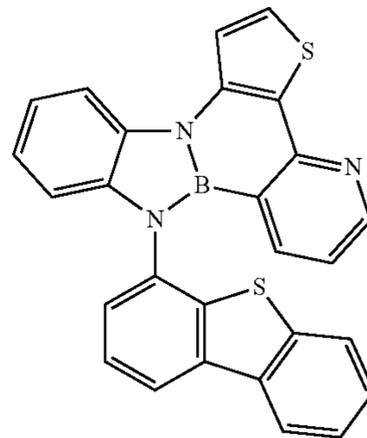


10

15

Compound 107

20

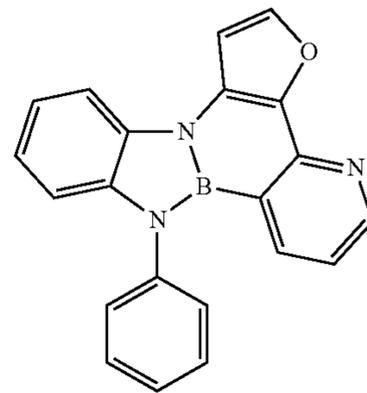


25

30

Compound 108

40

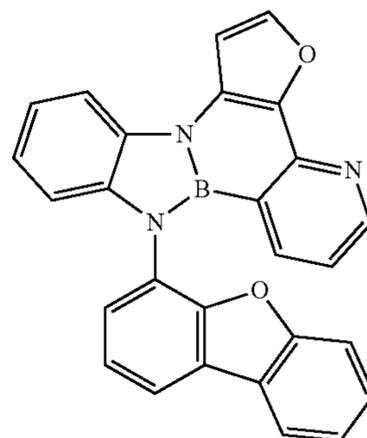


35

45

Compound 109

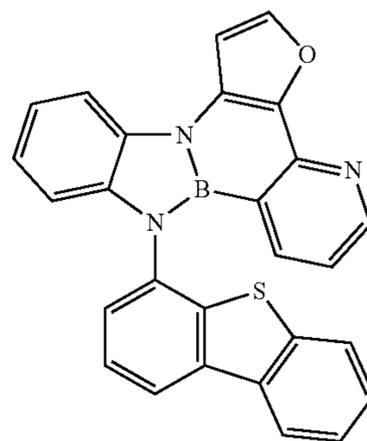
55



50

60

65



Compound 110

Compound 111

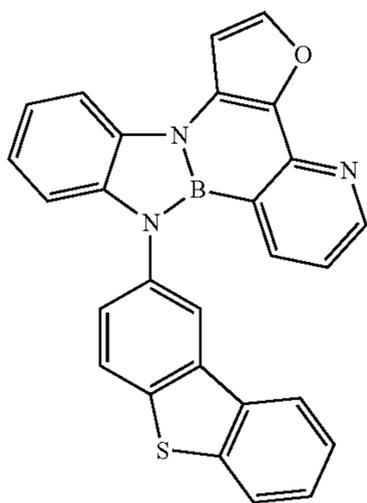
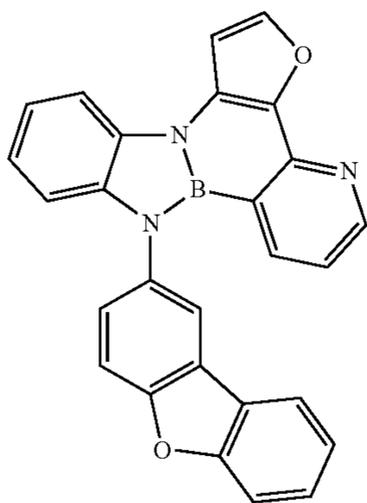
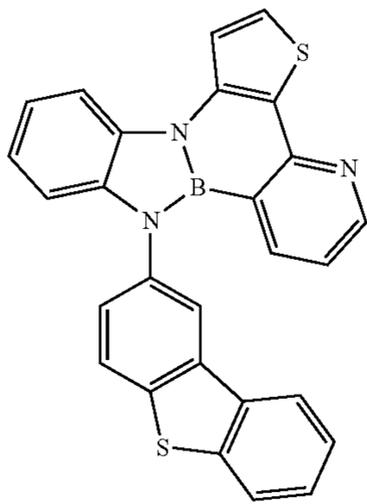
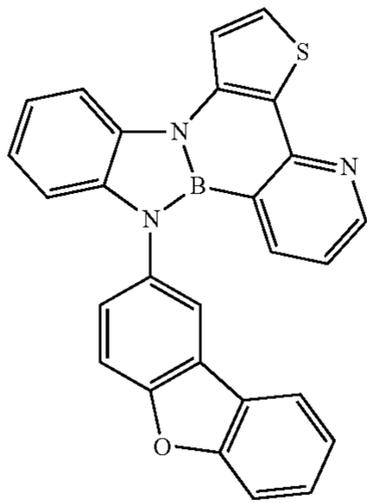
Compound 112

Compound 113

Compound 114

**23**

-continued



**24**

-continued

Compound 115

5

10

15

Compound 116

20

25

30

Compound 117

35

40

45

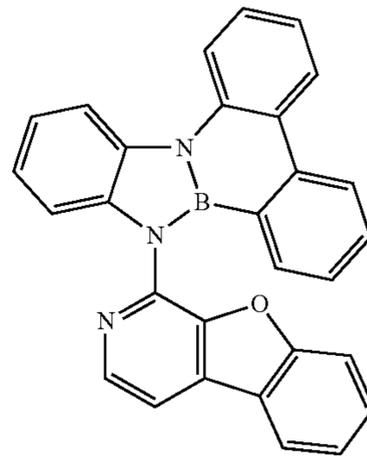
50

Compound 118

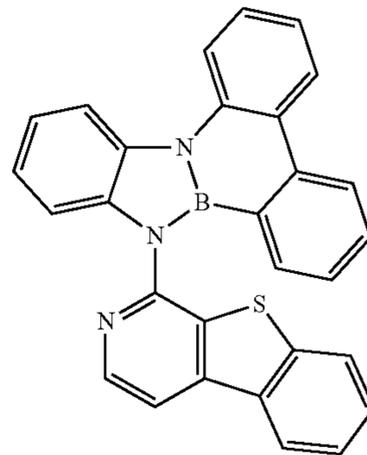
55

60

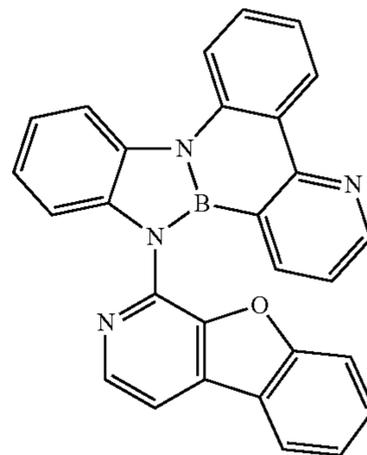
65



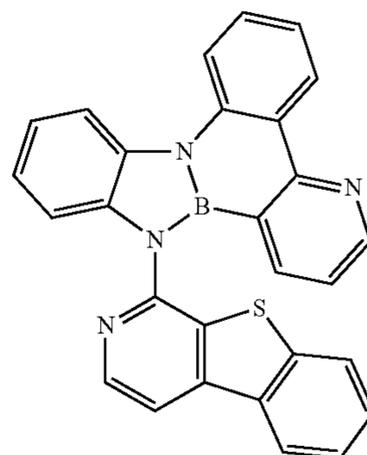
Compound 119



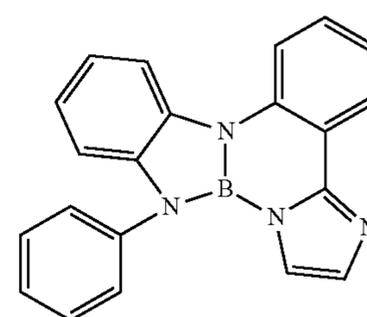
Compound 120



Compound 121



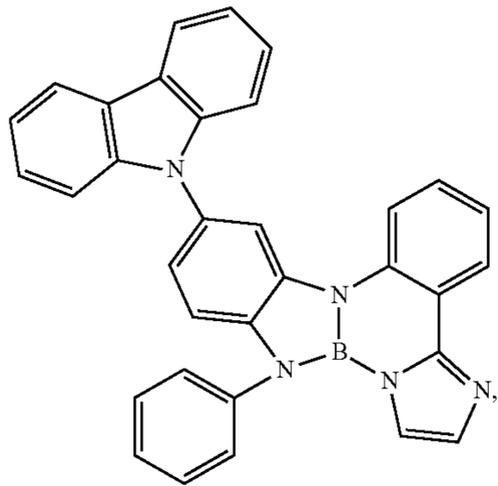
Compound 122



Compound 123

25

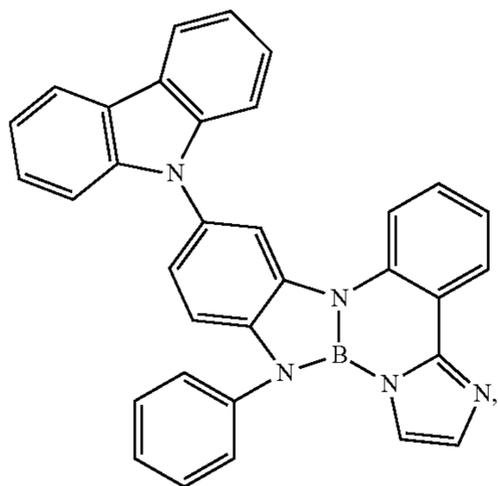
-continued



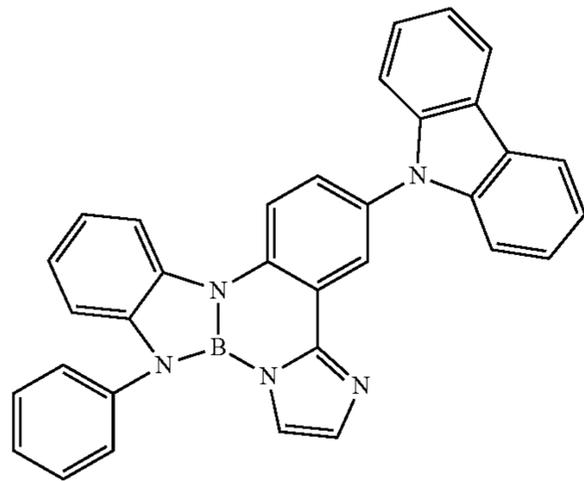
Compound 124

5

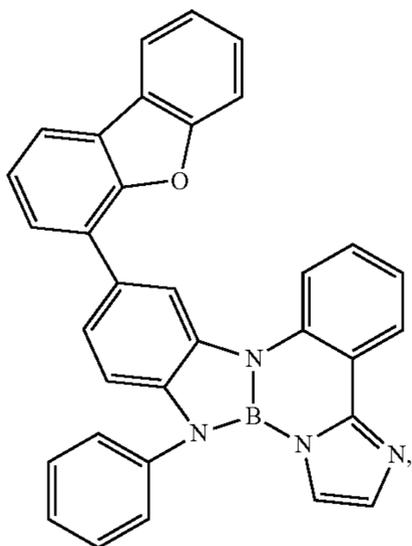
Compound 125



Compound 126

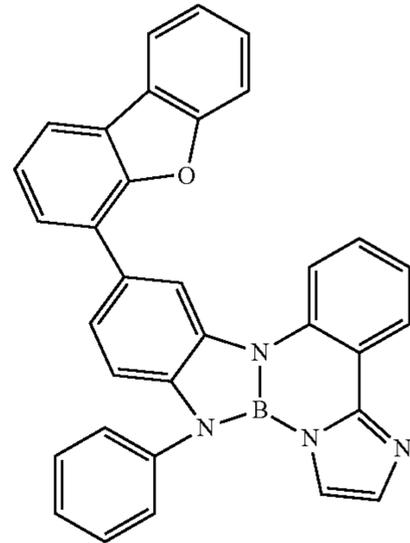


Compound 127



26

-continued



Compound 128

10

15

20

25

30

35

40

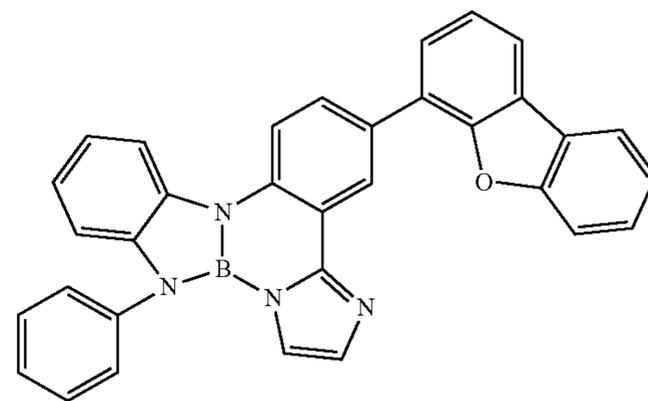
45

50

55

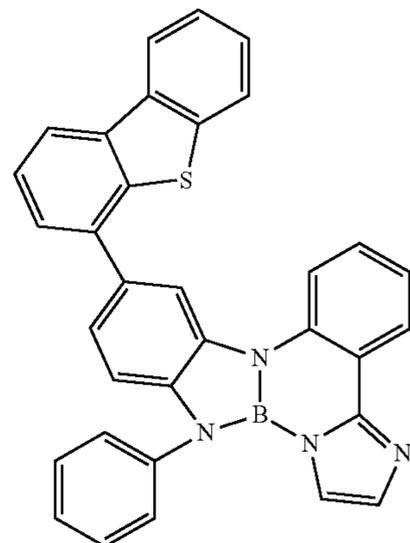
60

65

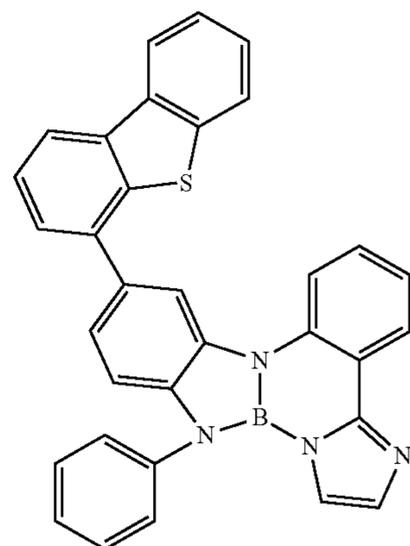


Compound 129

Compound 130



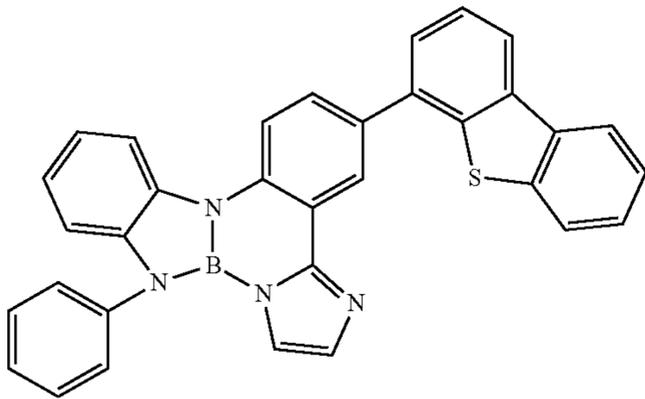
Compound 131



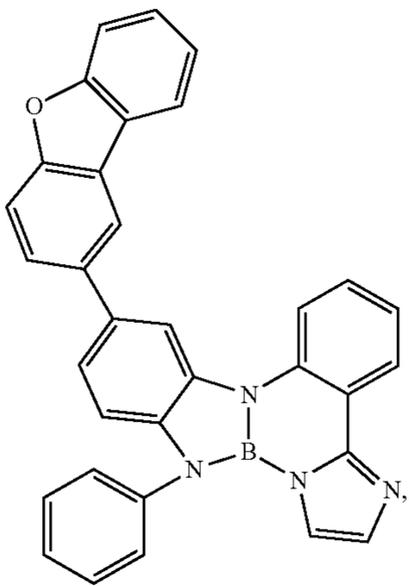
27

-continued

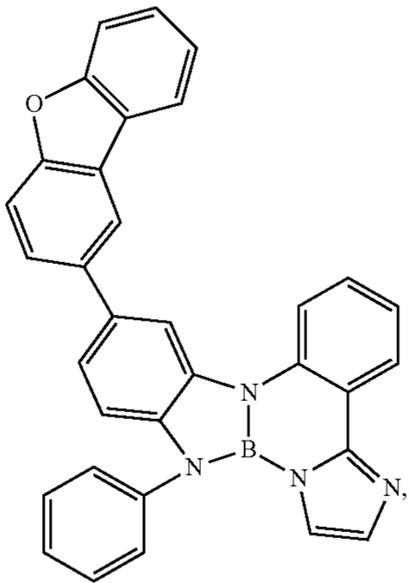
Compound 132



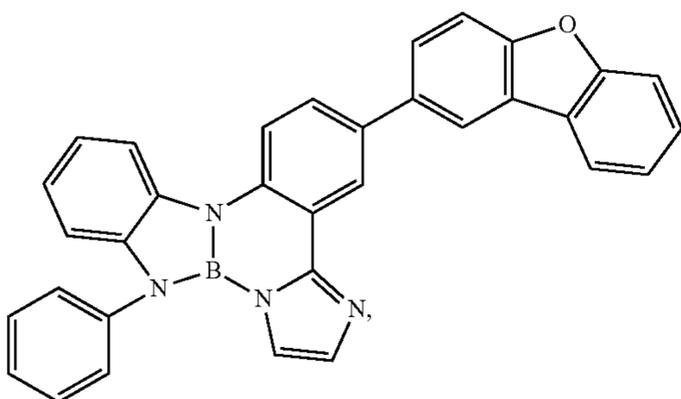
Compound 133



Compound 134



Compound 135

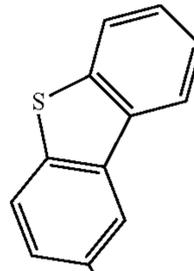


28

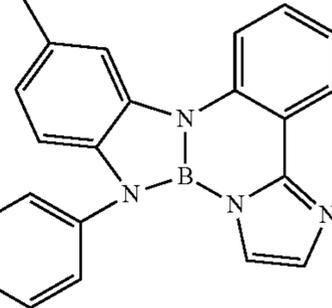
-continued

Compound 136

5



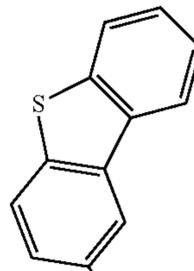
10



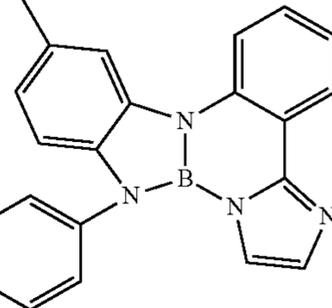
15

Compound 137

20



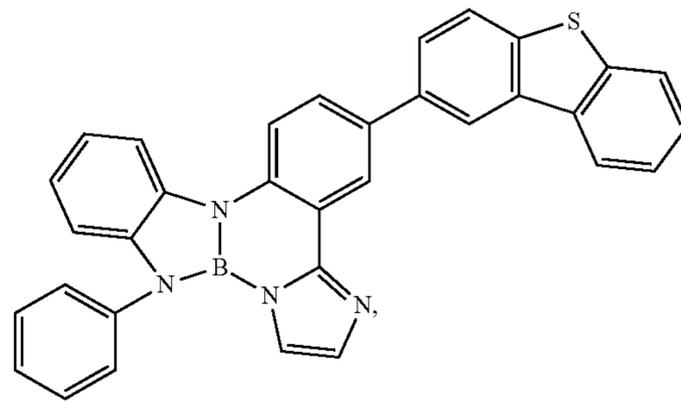
25



30

Compound 138

35



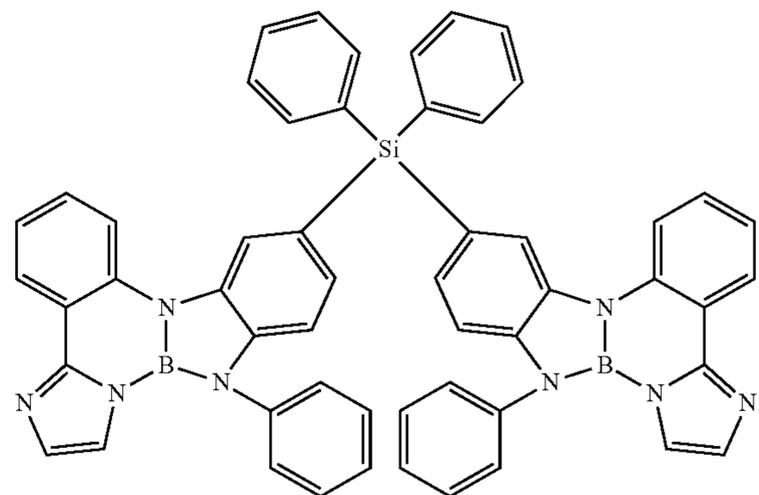
40

45

50

Compound 155

55



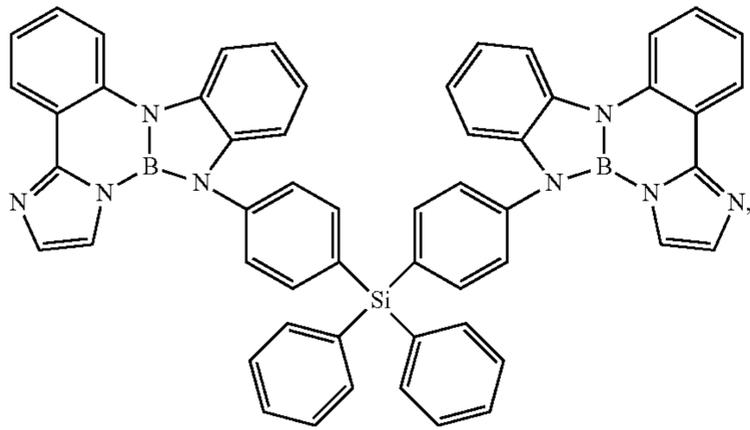
60

65

29

-continued

Compound 156

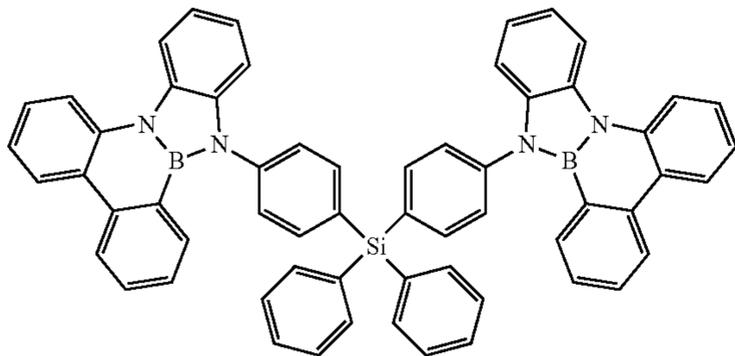


5

10

15

Compound 157

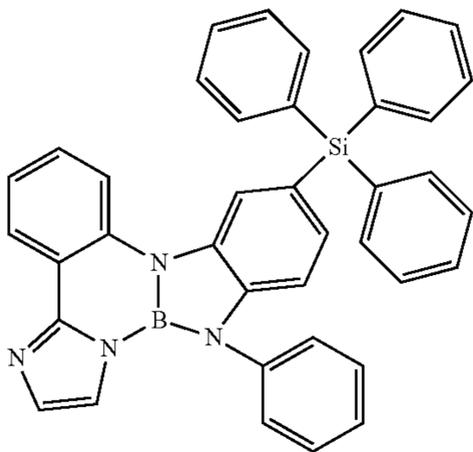


20

25

30

Compound 163



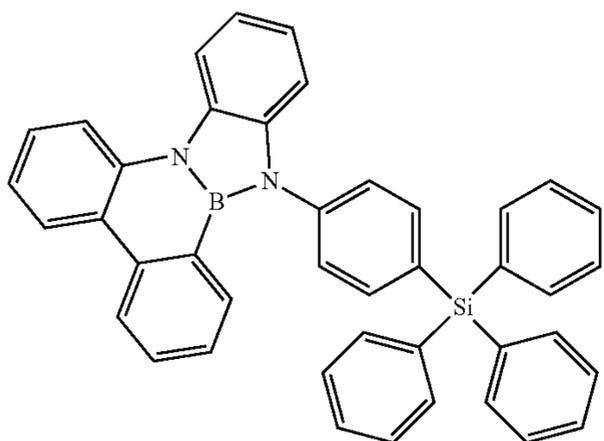
35

40

45

50

Compound 164



55

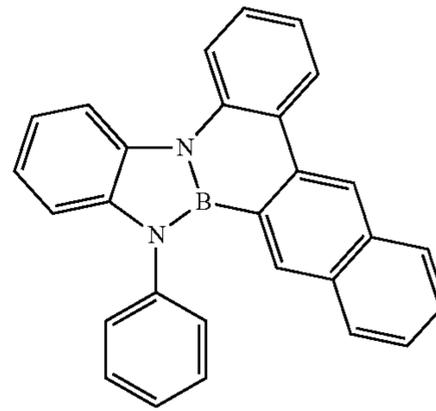
60

65

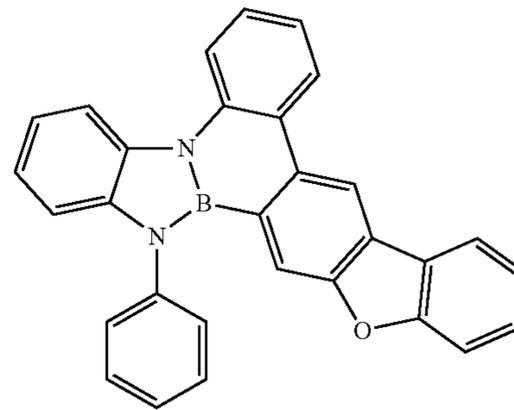
30

-continued

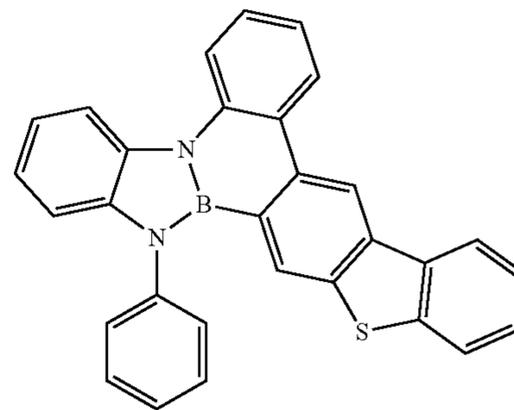
Compound 187



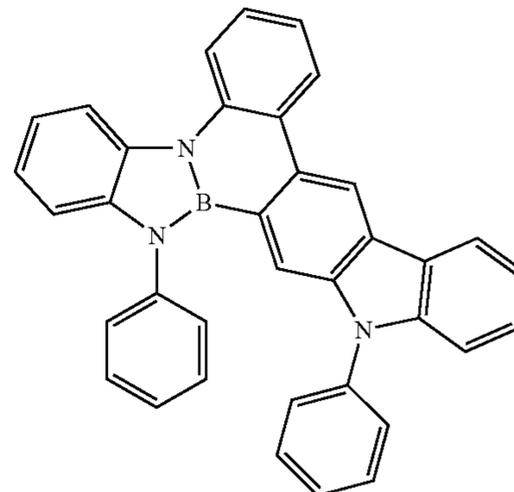
Compound 188



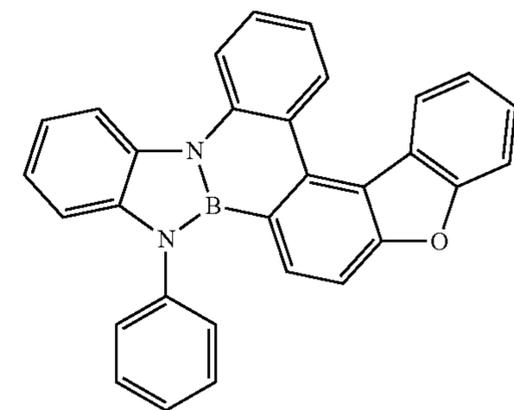
Compound 189



Compound 190

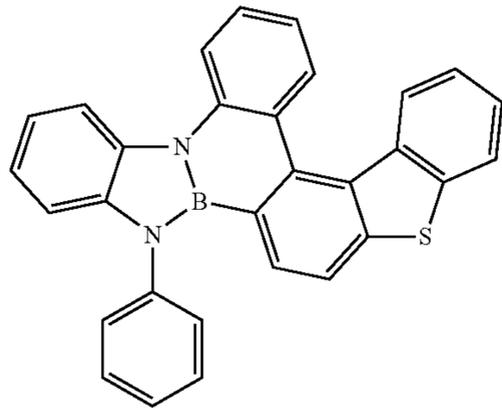


Compound 191



**31**

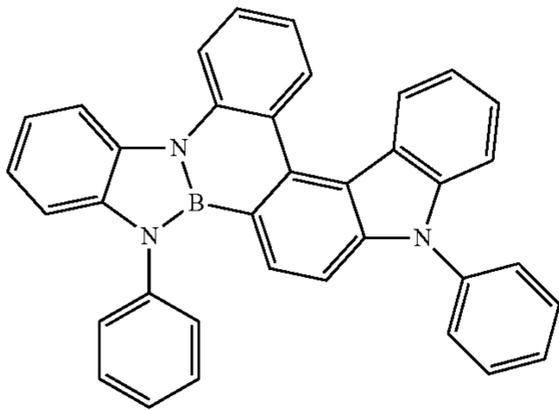
-continued



Compound 192

5

Compound 193

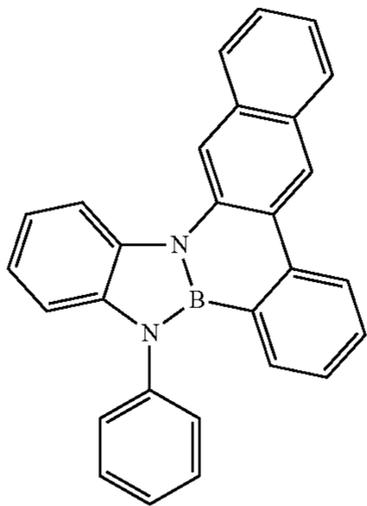


15

20

25

Compound 194



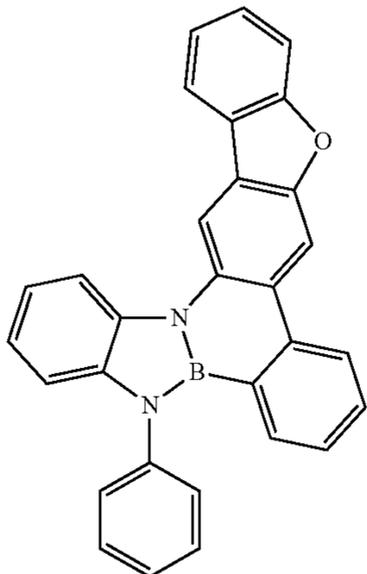
30

35

40

45

Compound 195



50

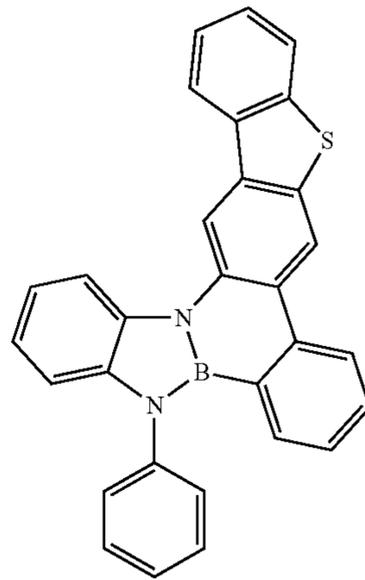
55

60

65

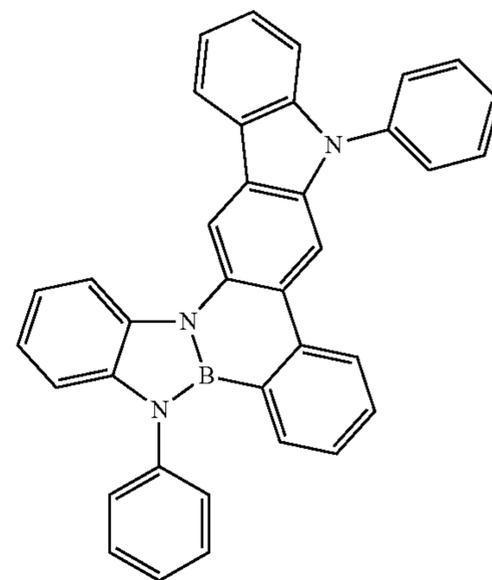
**32**

-continued

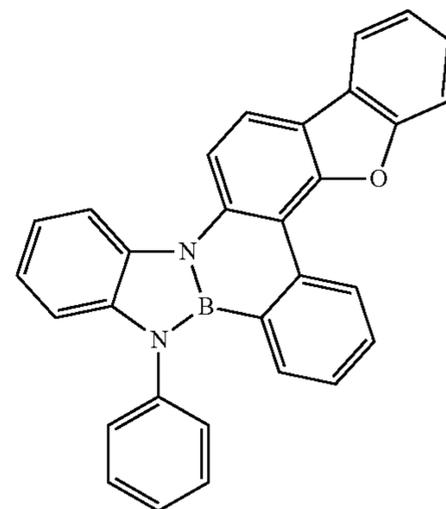


Compound 196

Compound 197

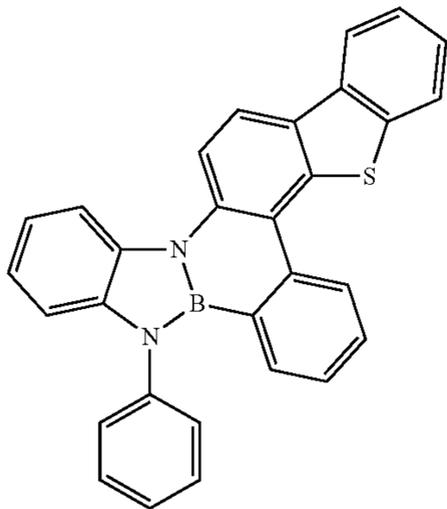


Compound 198



33

-continued



Compound 199

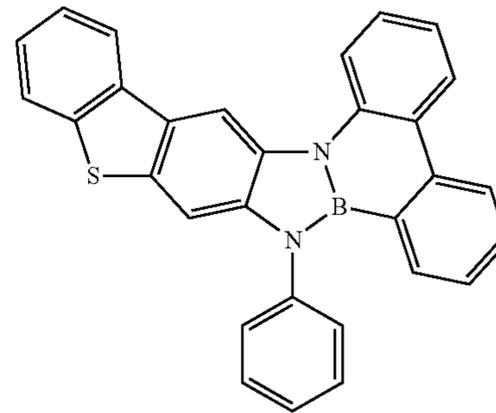
5

10

15

34

-continued



Compound 203

20

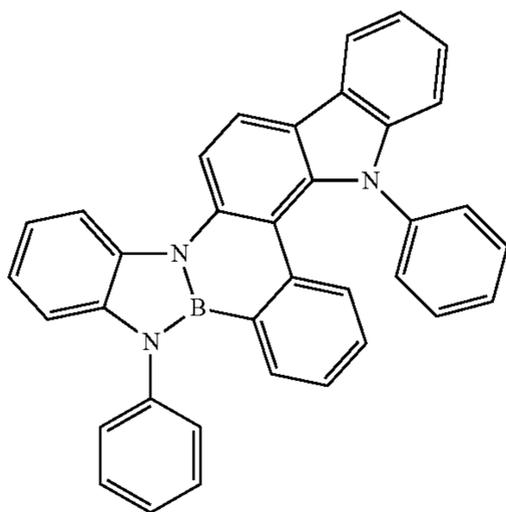
Compound 200

25

30

35

Compound 204



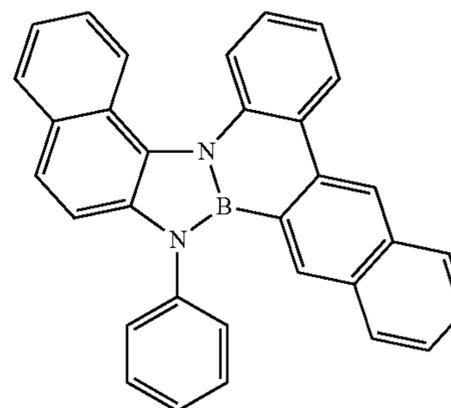
Compound 201

40

45

50

Compound 205



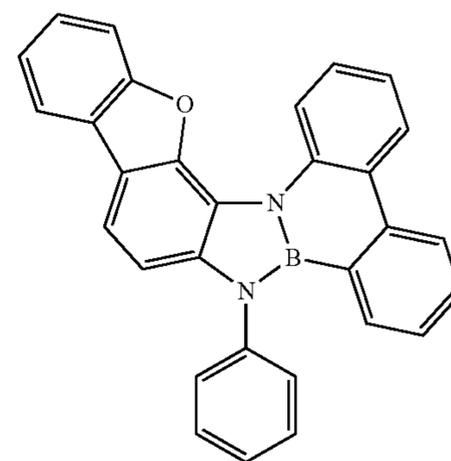
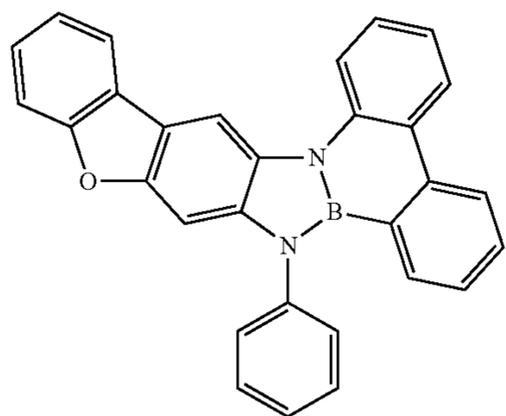
Compound 202

55

60

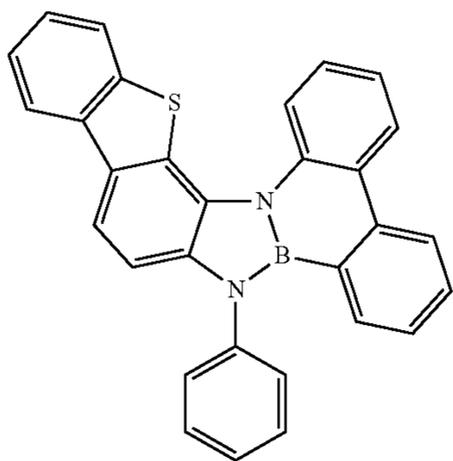
65

Compound 206



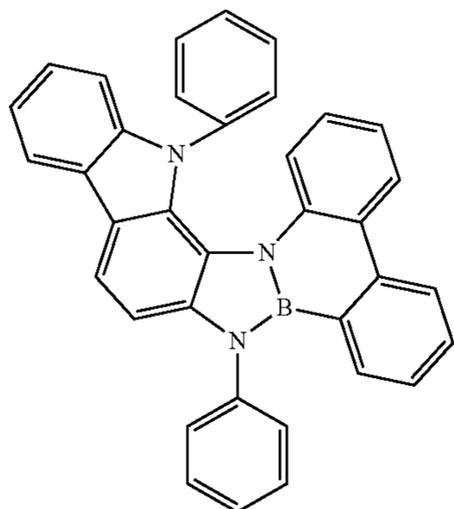
35

-continued



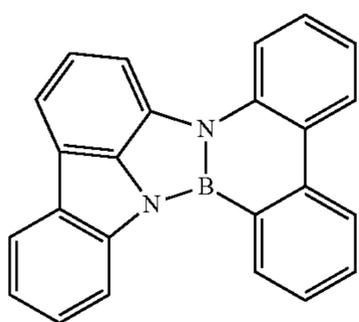
Compound 207

, and

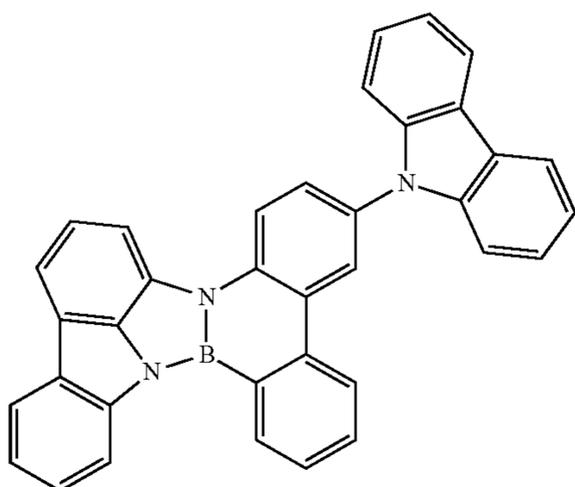


Compound 208

In some embodiments,  $X^1$  is C or N, A is aryl or heteroaryl and A is connected to  $X^1$  to form a fused ring. In some such embodiments, the compound is selected from the group consisting of:



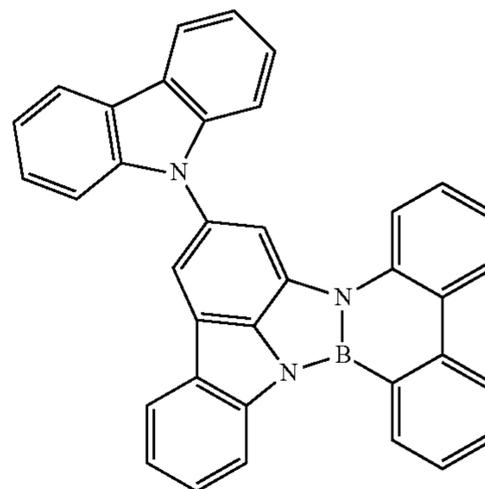
Compound 1



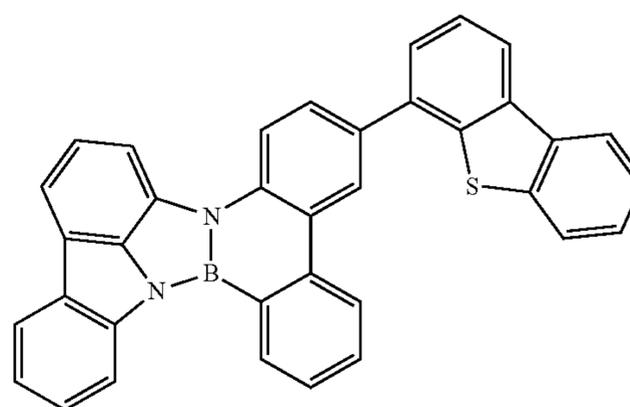
Compound 2

36

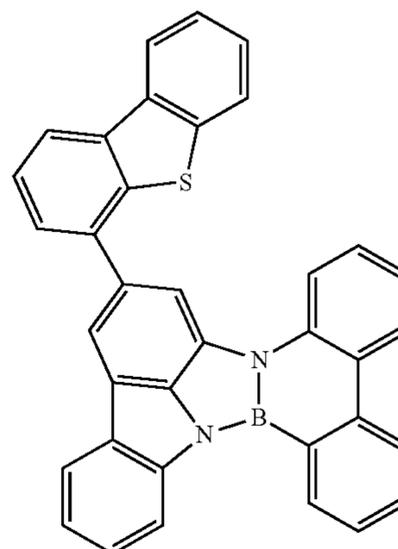
-continued



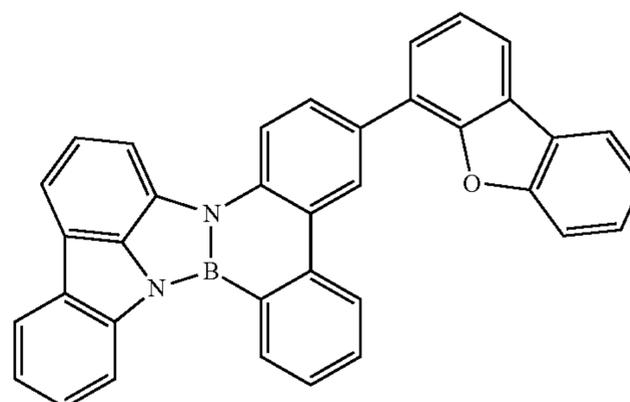
Compound 3



Compound 4



Compound 5



Compound 6

5

10

15

20

25

30

35

40

45

50

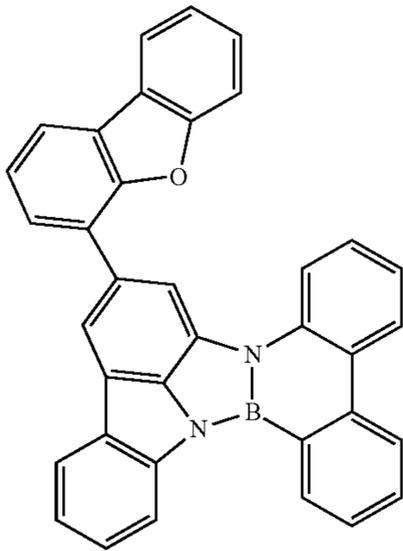
55

60

65

37

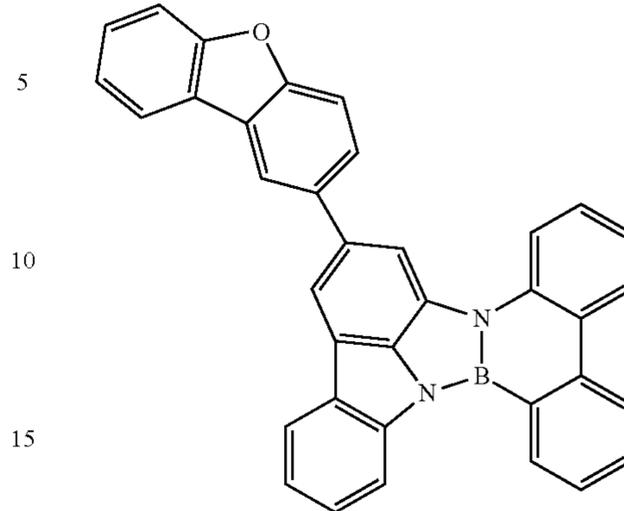
-continued



Compound 7

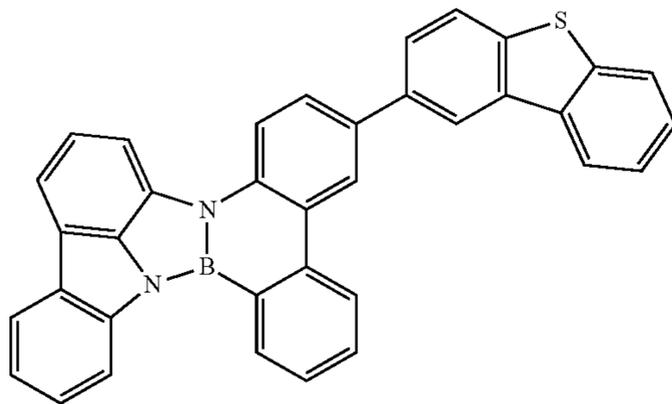
38

-continued

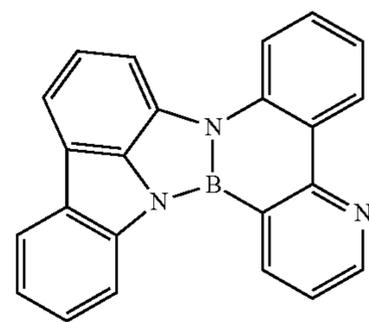


Compound 11

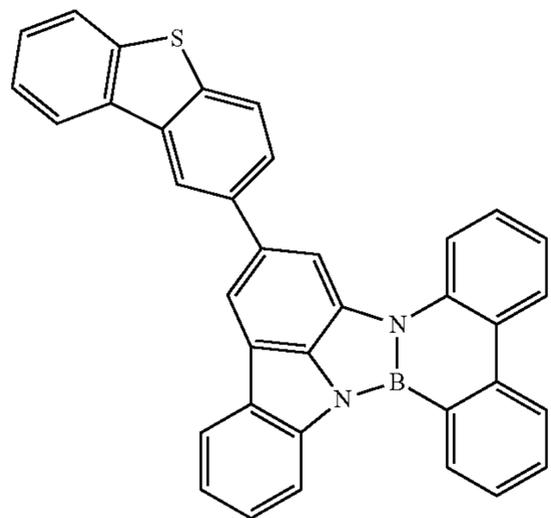
Compound 8



Compound 12

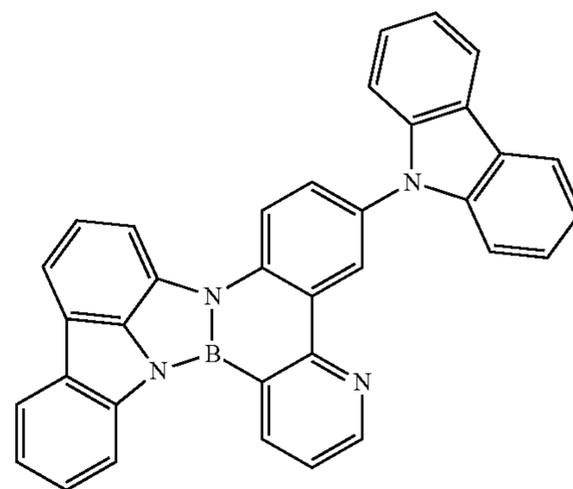


Compound 9



Compound 13

Compound 13

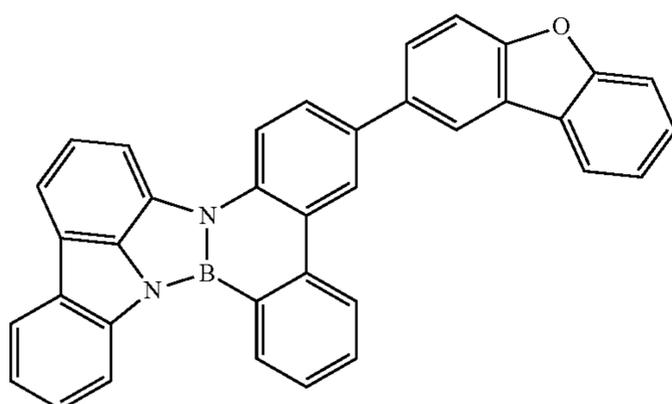


Compound 14

Compound 14

Compound 14

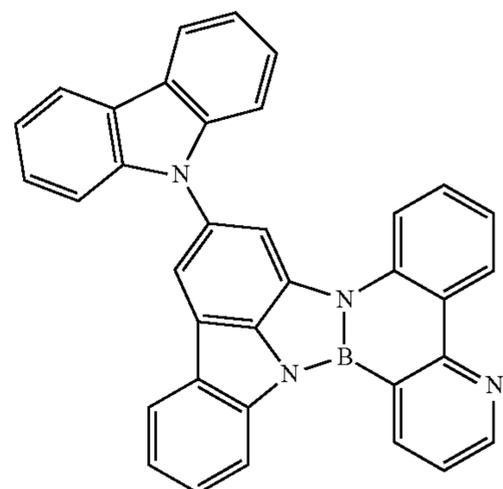
Compound 10



Compound 14

Compound 14

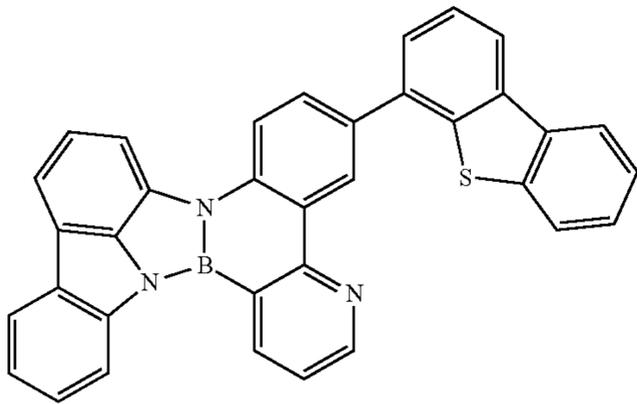
Compound 14



39

-continued

Compound 15

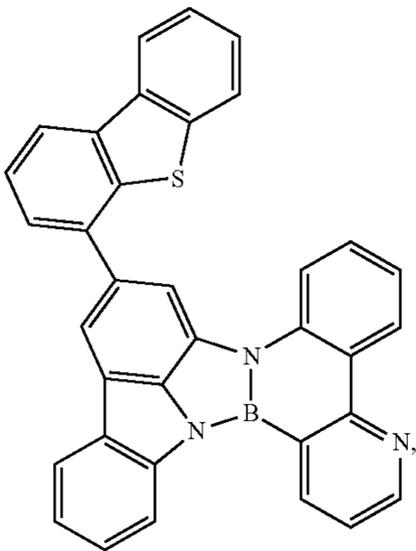


5

10

15

Compound 16



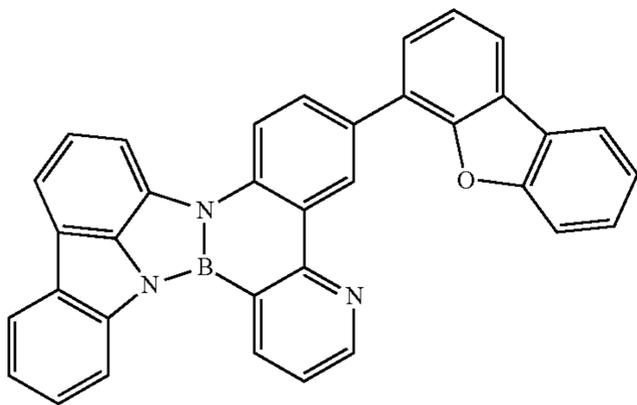
20

25

30

Compound 17

35

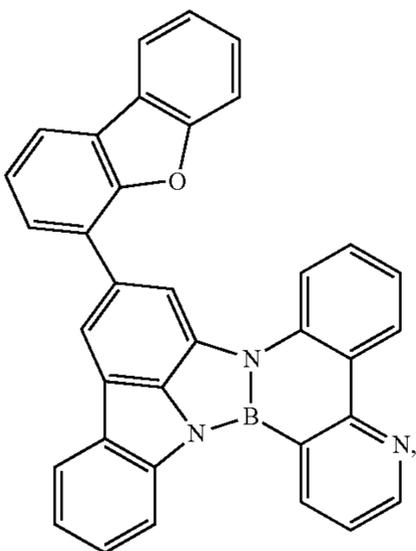


40

45

Compound 18

50



55

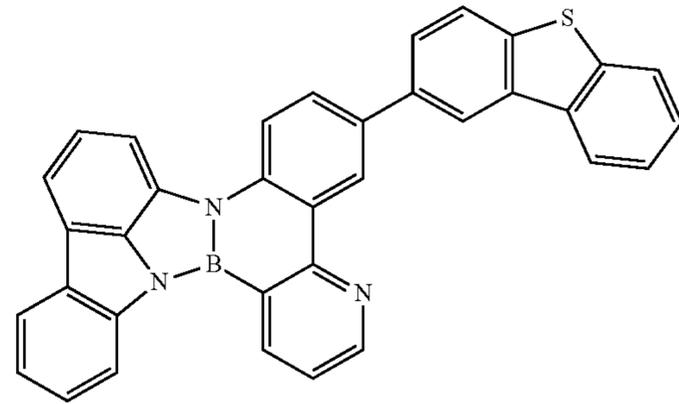
60

65

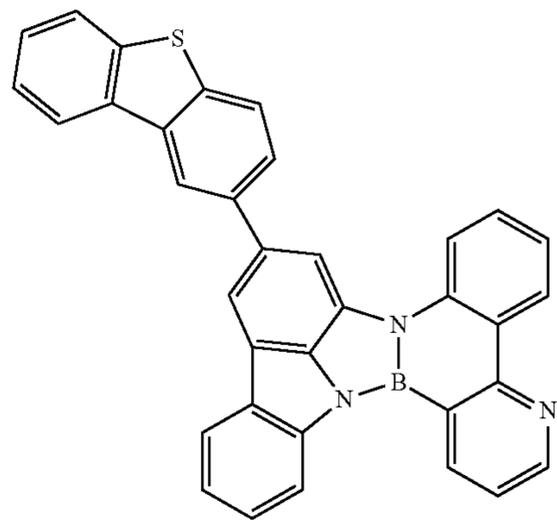
40

-continued

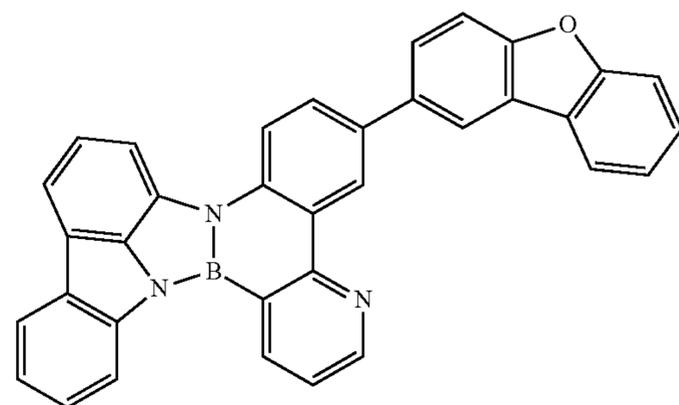
Compound 19



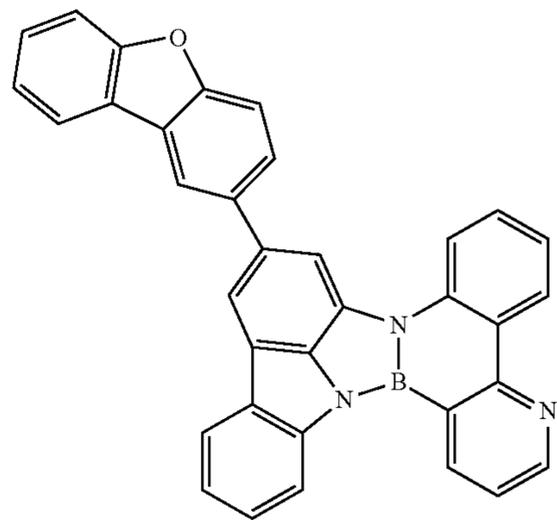
Compound 20



Compound 21

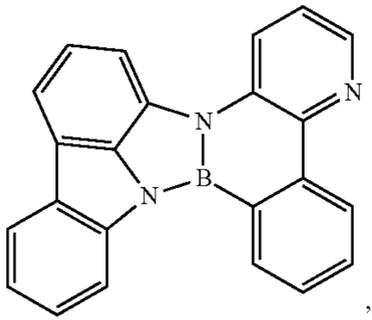


Compound 22



41

-continued

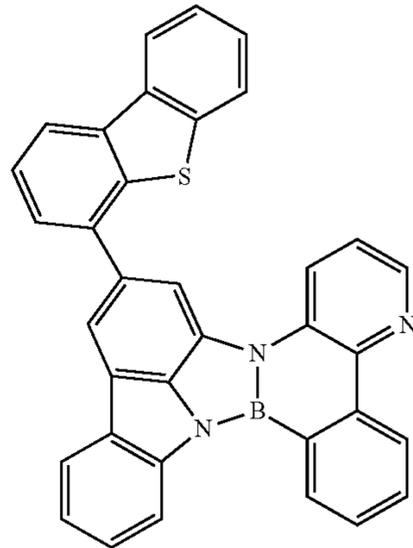


Compound 23

5

42

-continued



Compound 24

10

15

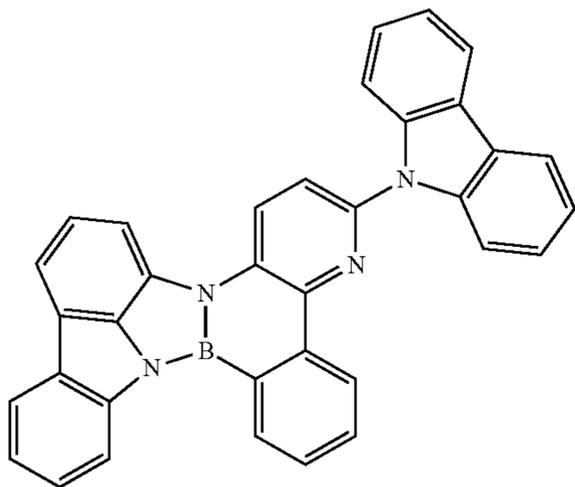
Compound 27

20

25

30

Compound 28



Compound 25

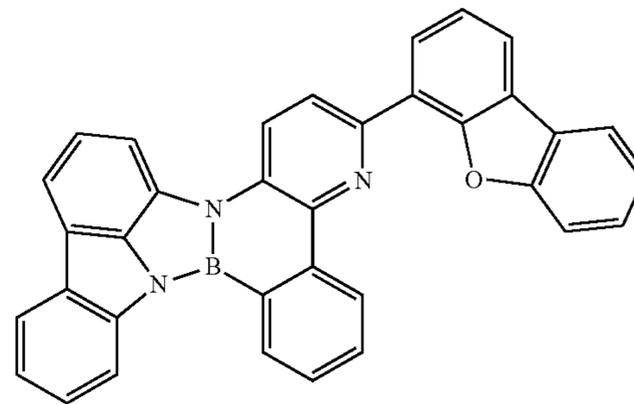
35

40

45

50

Compound 29



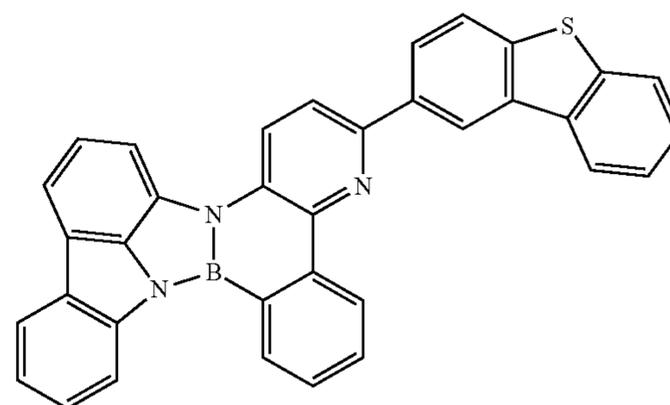
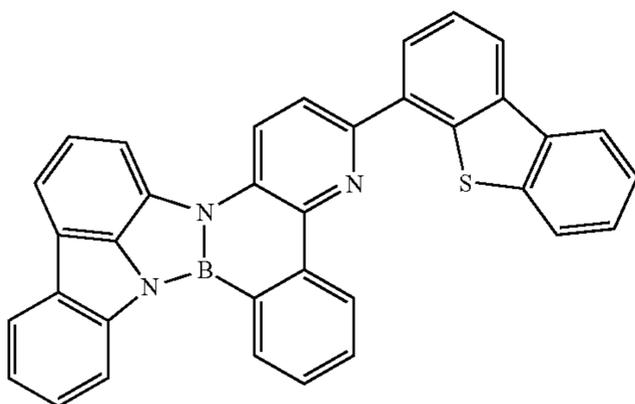
Compound 26

55

60

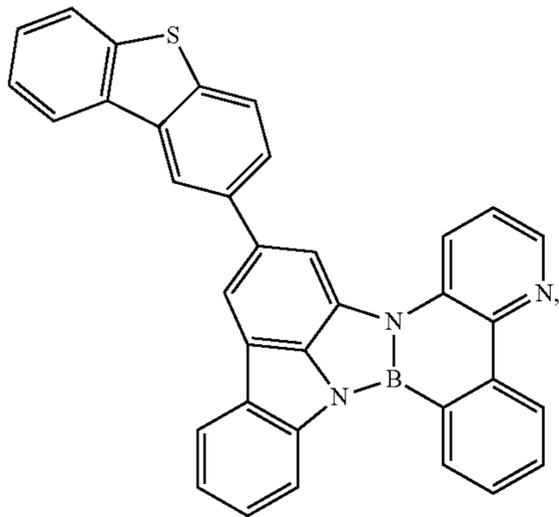
65

Compound 30



43

-continued

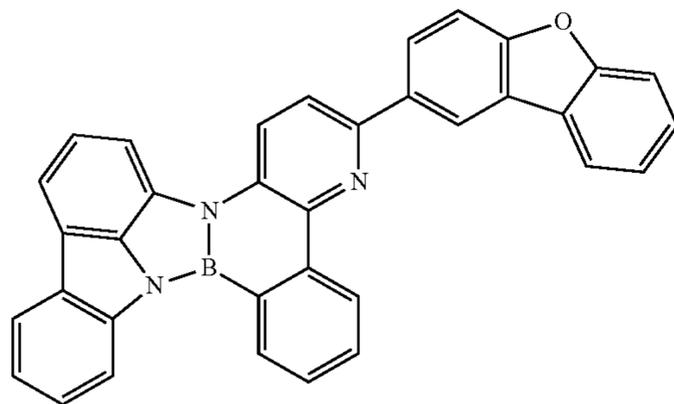


Compound 31

5

10

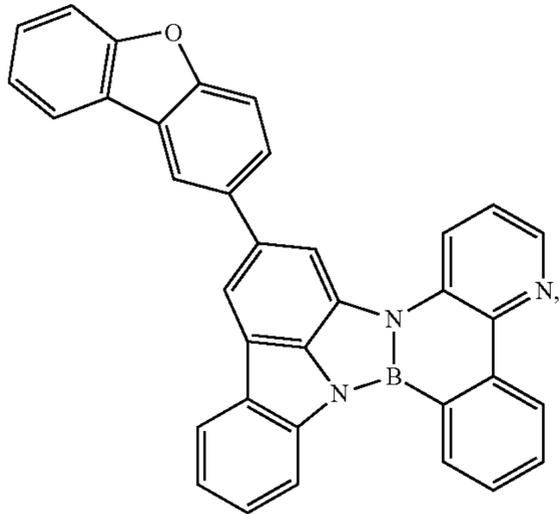
Compound 32



20

25

Compound 33

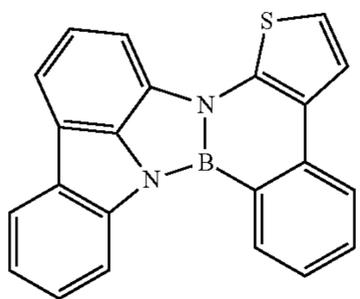


35

40

45

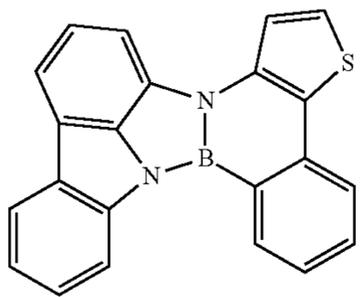
Compound 49



50

55

Compound 50

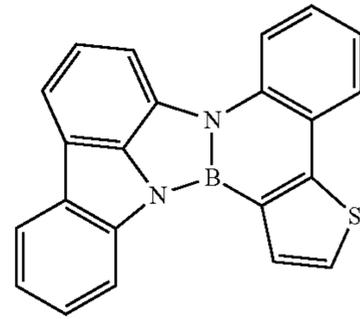


60

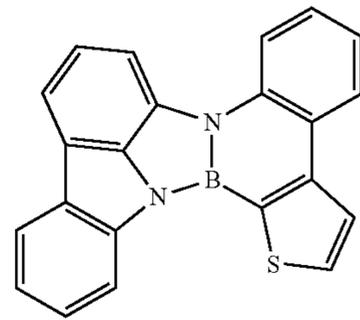
65

44

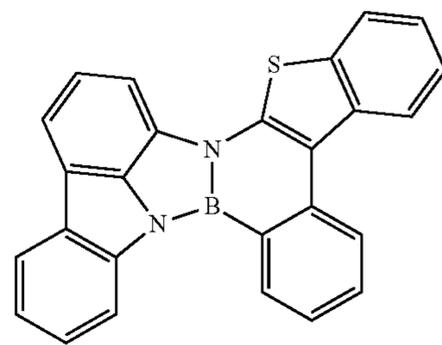
-continued



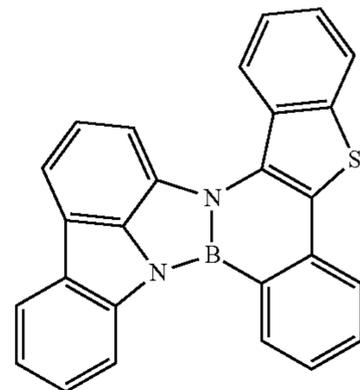
Compound 51



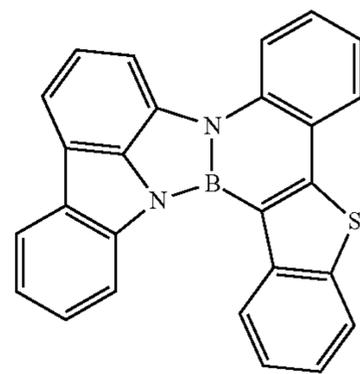
Compound 52



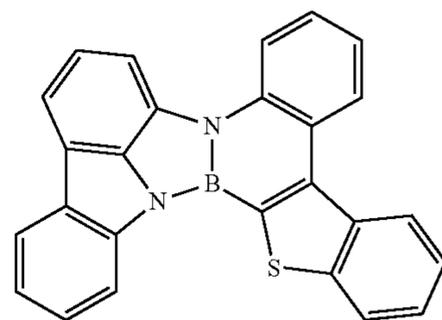
Compound 53



Compound 54



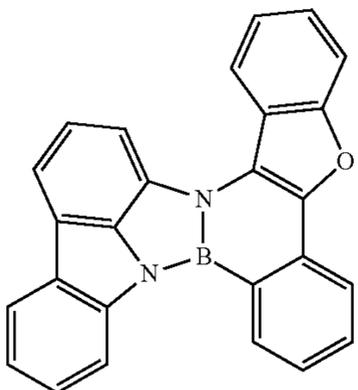
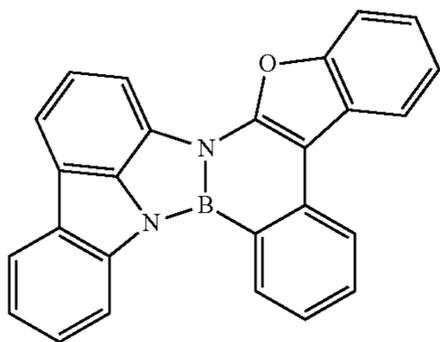
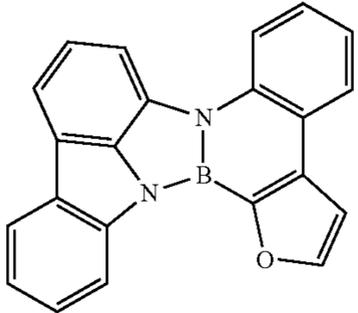
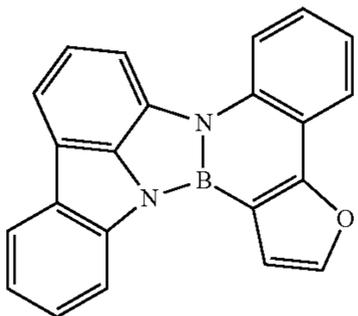
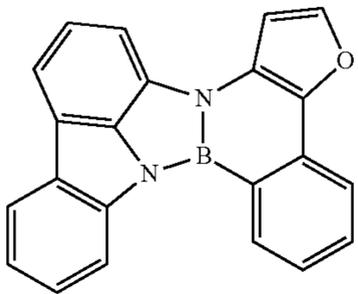
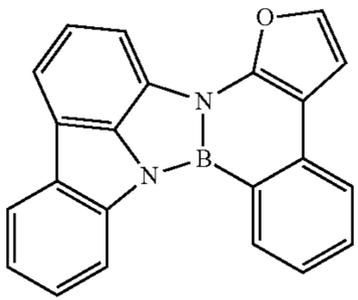
Compound 55



Compound 56

45

-continued

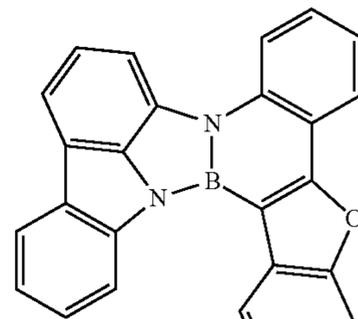


46

-continued

Compound 57

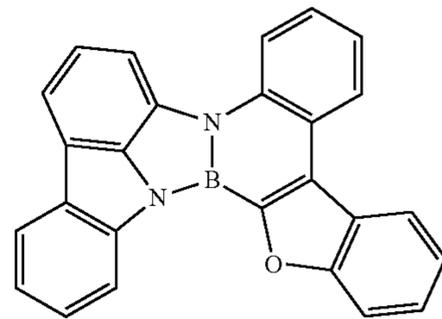
5



10

Compound 58

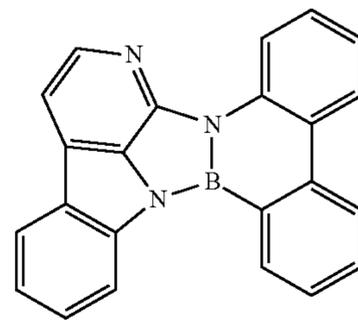
15



20

Compound 59

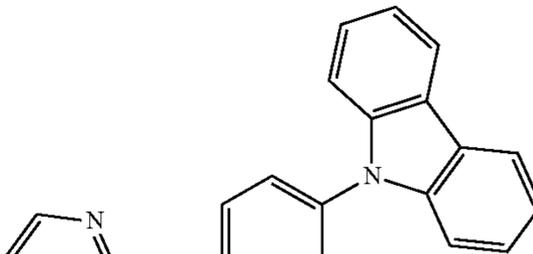
25



30

Compound 60

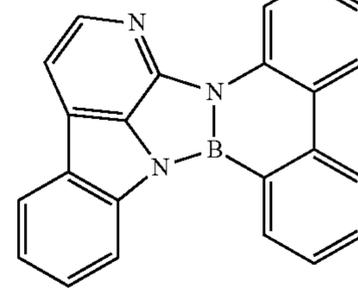
35



40

Compound 61

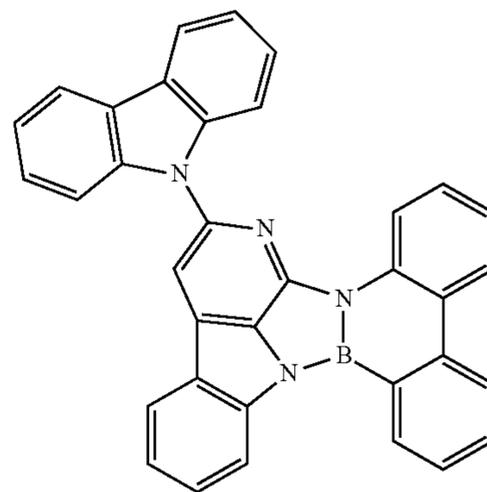
45



50

Compound 62

55



60

65

Compound 63

Compound 64

Compound 65

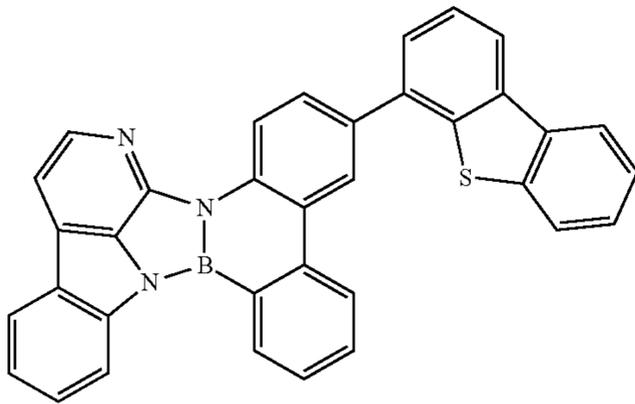
Compound 66

Compound 67

47

-continued

Compound 68

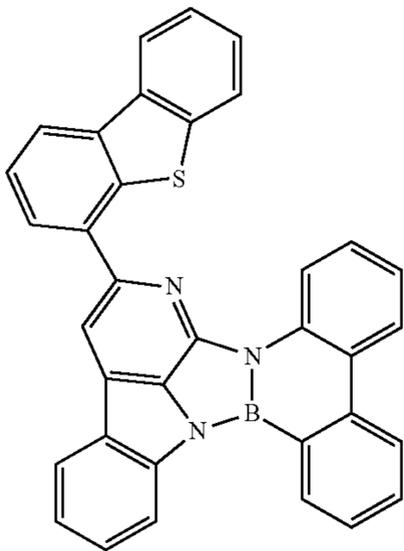


5

10

15

Compound 69

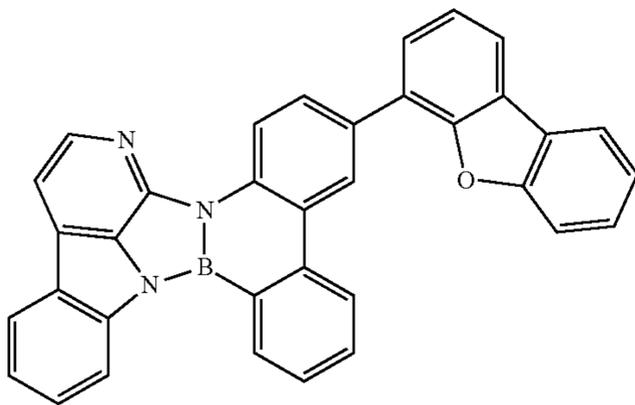


20

25

30

Compound 70

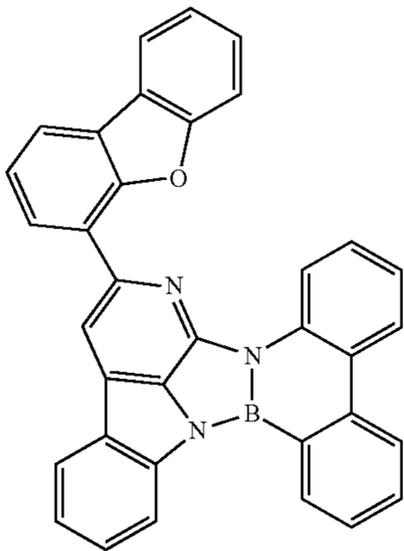


35

40

45

Compound 71



50

55

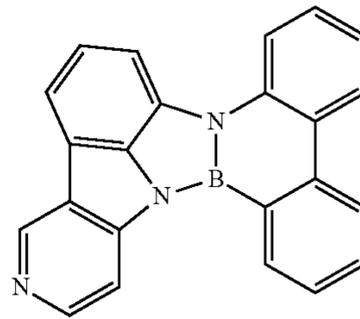
60

65

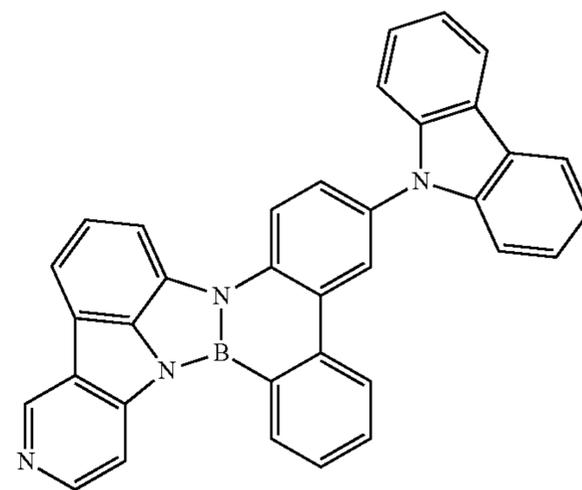
48

-continued

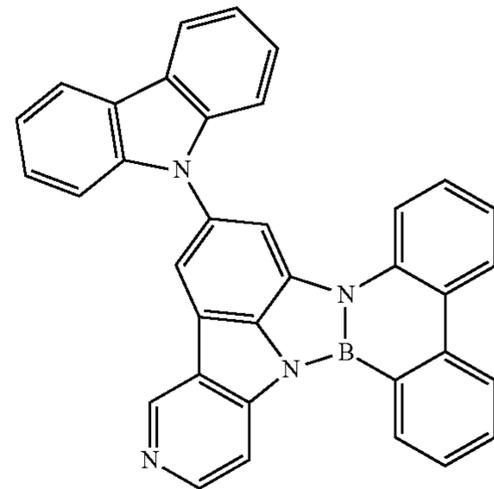
Compound 72



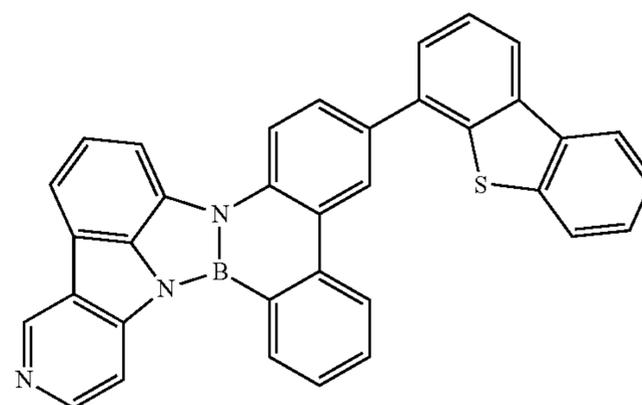
Compound 73



Compound 74

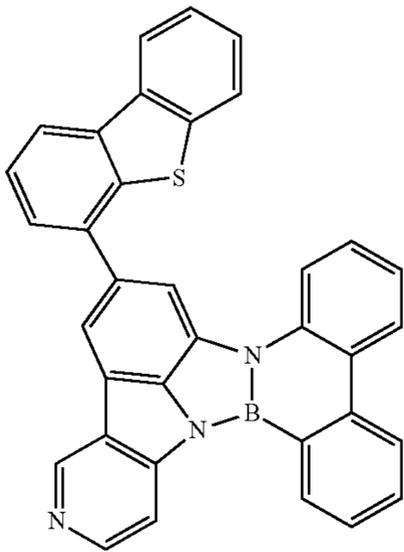


Compound 75

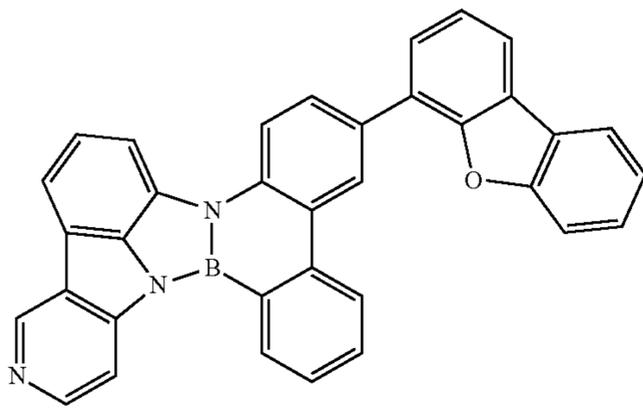


49

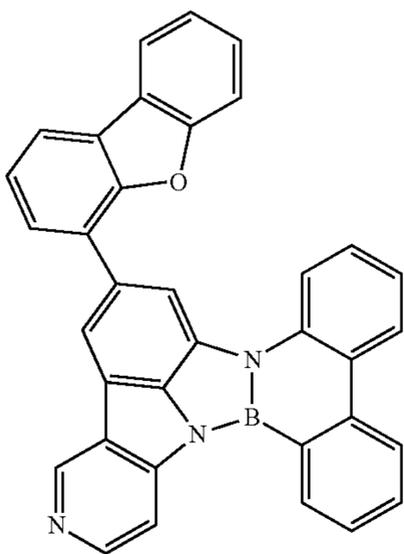
-continued



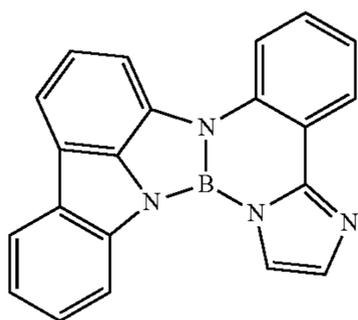
Compound 76



Compound 77



Compound 78

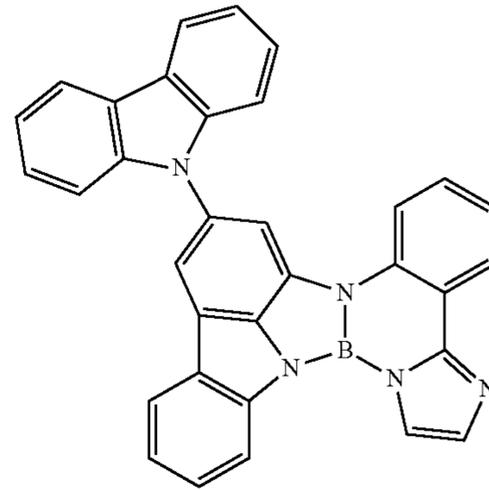


Compound 139

50

-continued

5



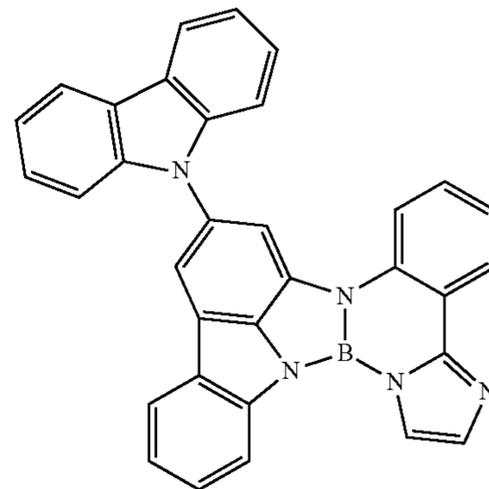
Compound 140

10

15

Compound 141

20

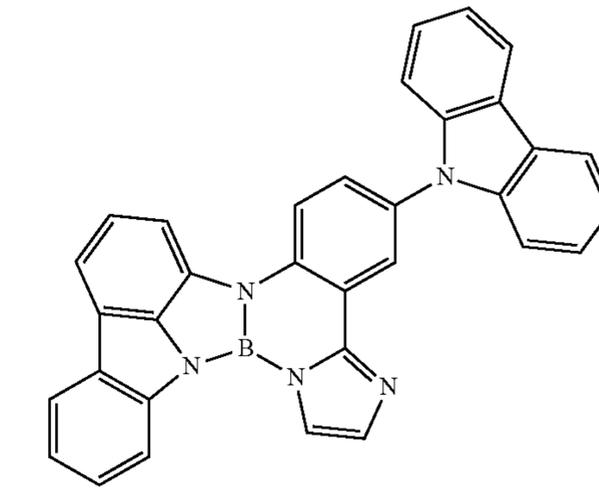


Compound 142

25

30

35



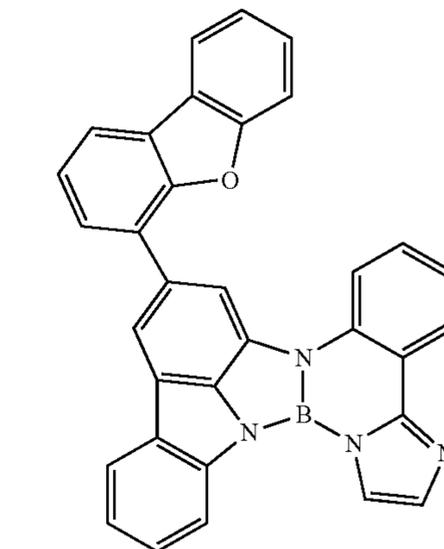
Compound 143

40

45

50

55



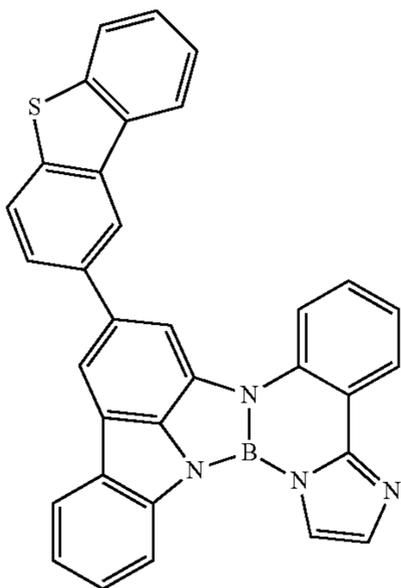
60

65



53

-continued

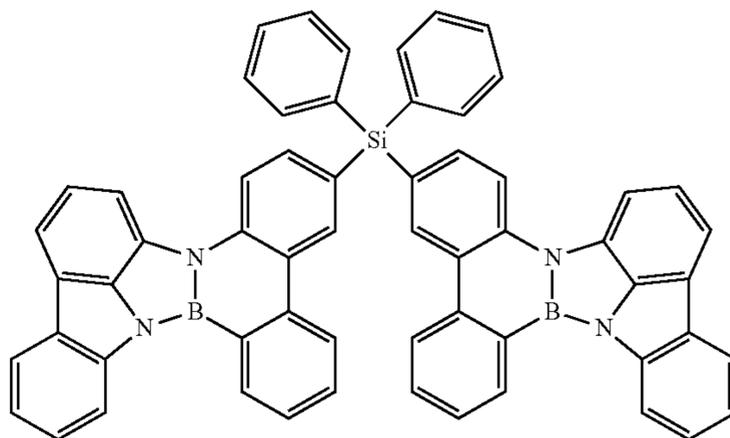


Compound 152

5

54

-continued

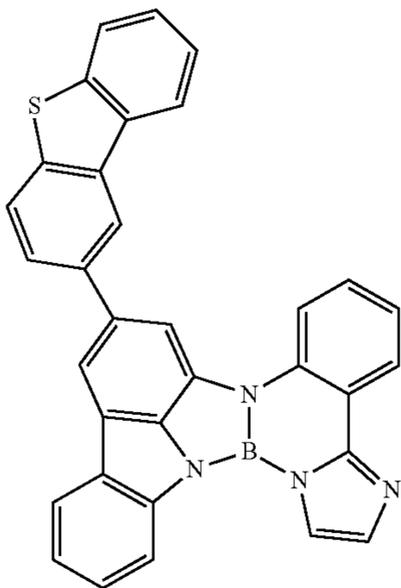


Compound 160

10

15

Compound 153

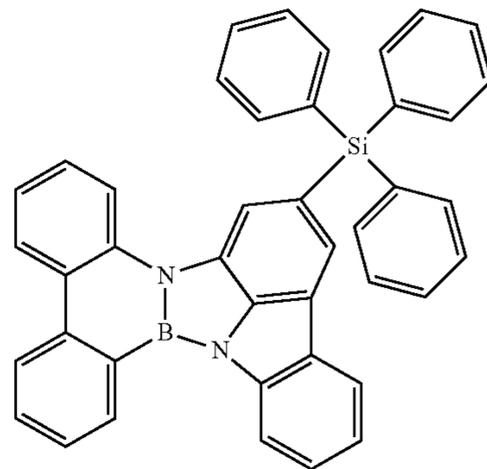


20

25

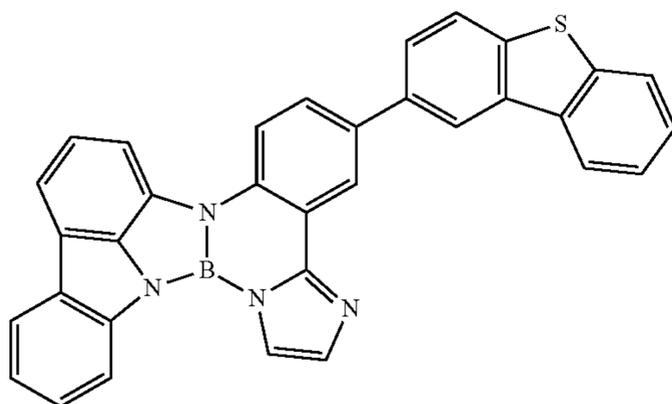
30

35



Compound 161

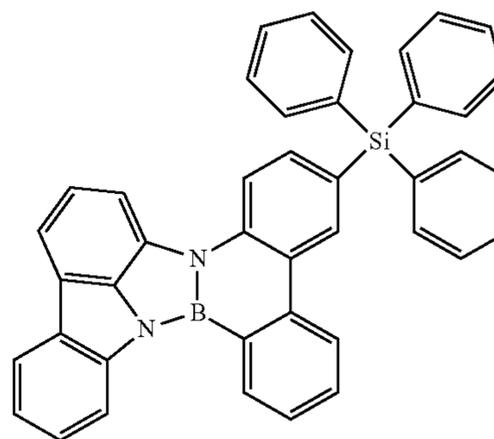
Compound 154



40

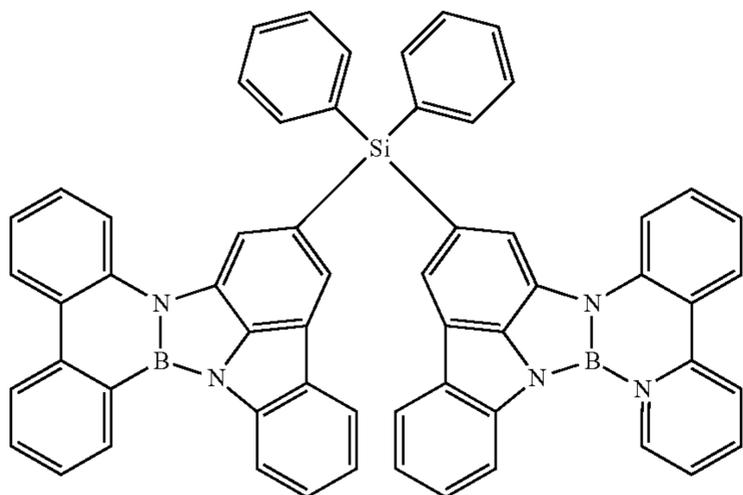
45

50



Compound 162

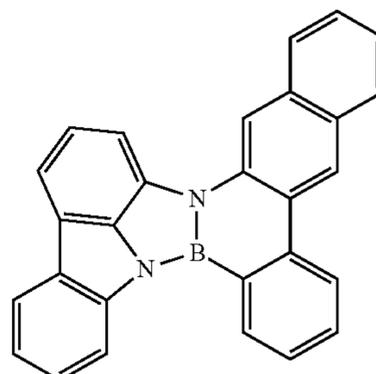
Compound 159



55

60

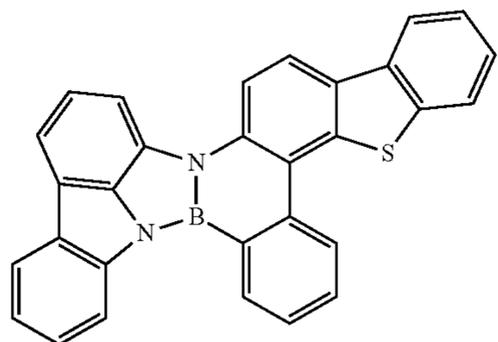
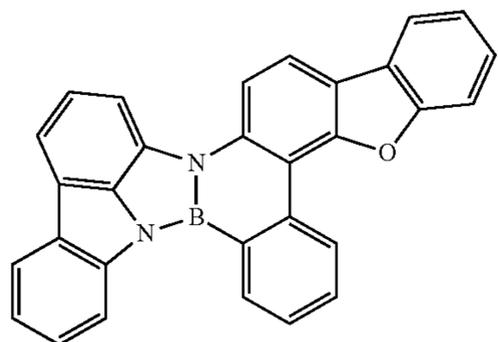
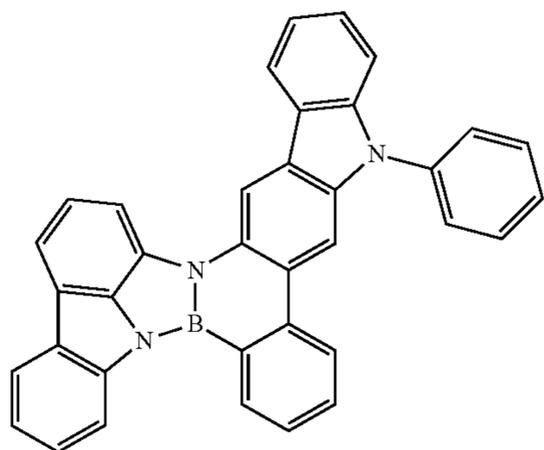
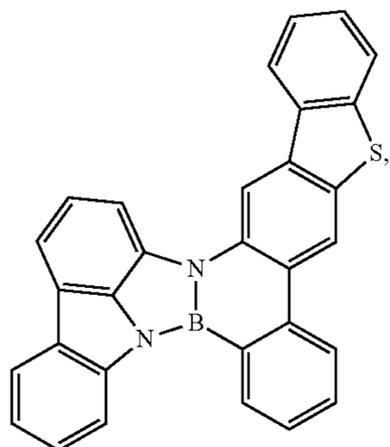
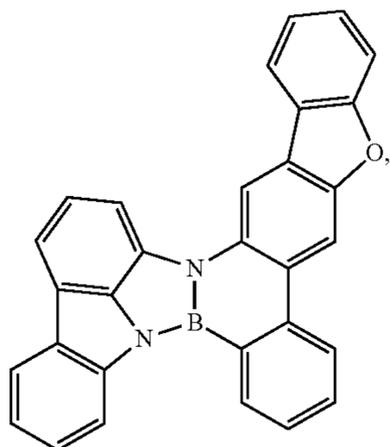
65



Compound 165

**55**

-continued

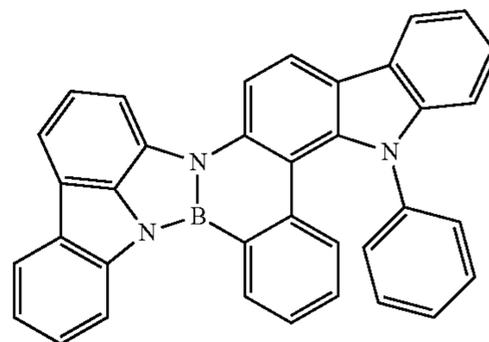


**56**

-continued

Compound 166

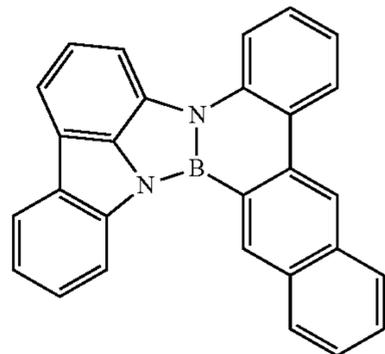
5



10

Compound 167

15

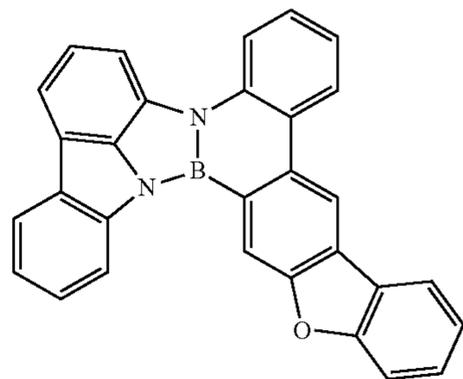


20

25

Compound 168

30

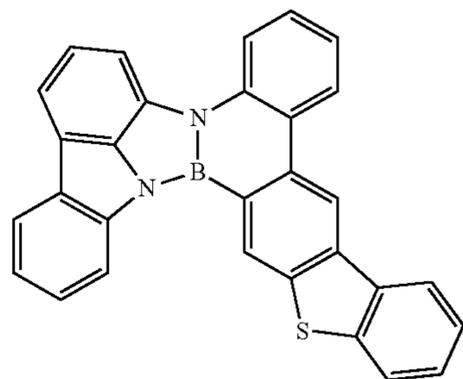


35

40

Compound 169

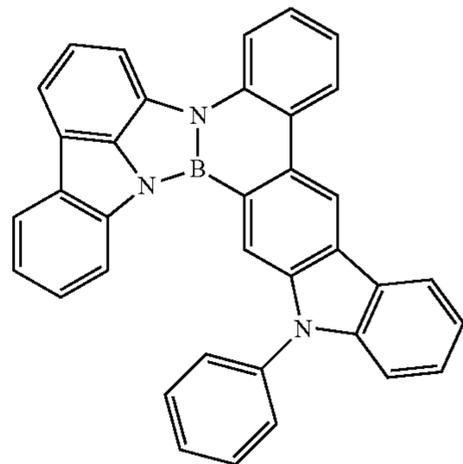
45



50

Compound 170

55



60

65

Compound 171

Compound 172

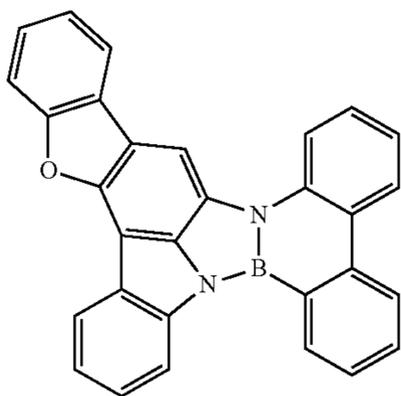
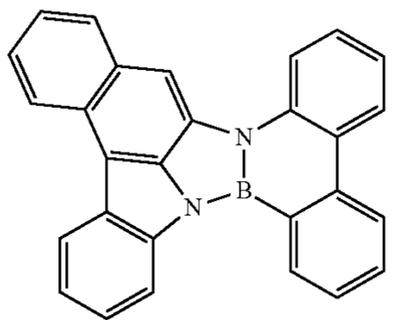
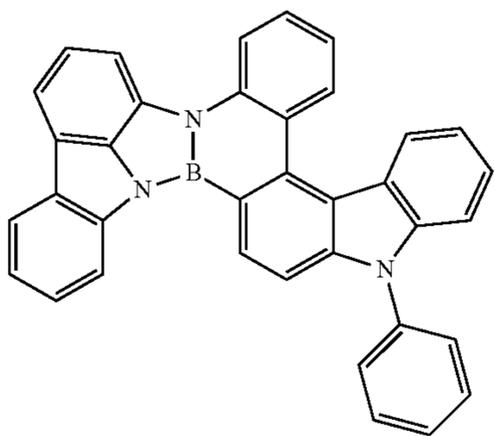
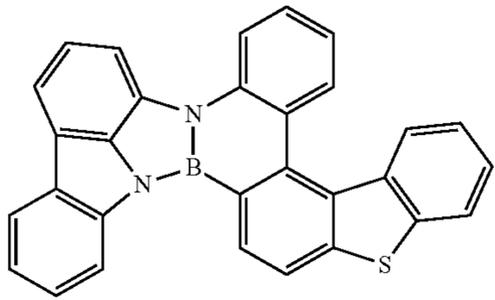
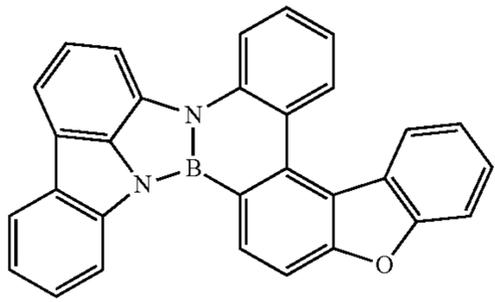
Compound 173

Compound 174

Compound 175

57

-continued



58

-continued

Compound 176

5

10

Compound 177

15

20

Compound 178

25

30

35

40

Compound 179

45

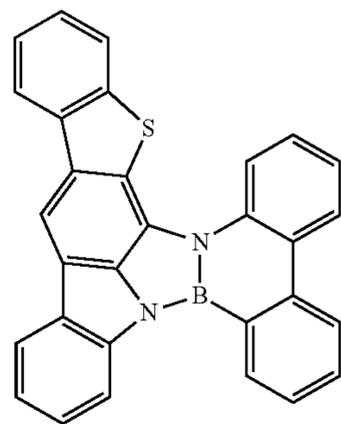
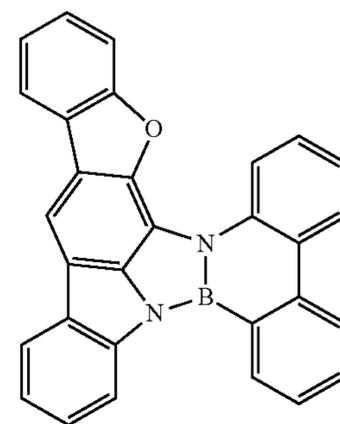
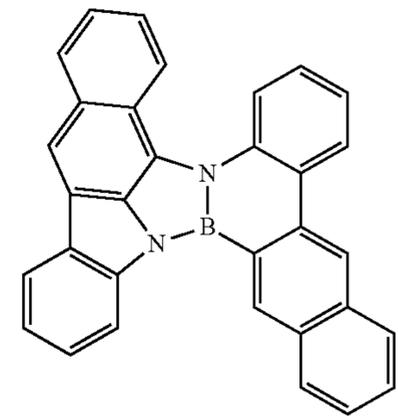
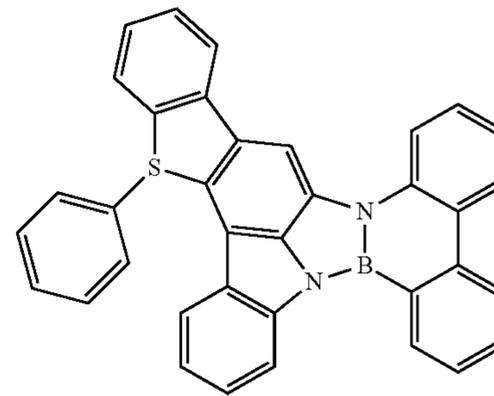
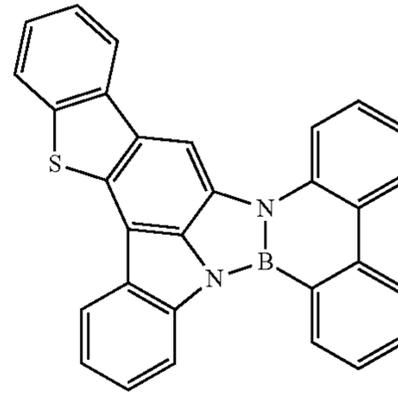
50

Compound 180

55

60

65



Compound 181

Compound 182

Compound 183

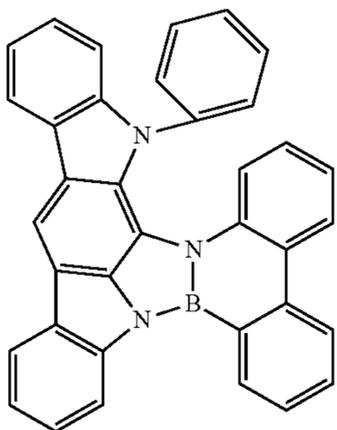
Compound 184

Compound 185

and

59

-continued



In some embodiments,  $R^A$  is an aryl ring. In some embodiments,  $R^A$  is benzene.

In some embodiments,  $R^B$  is an aryl ring or a heteroaryl ring comprising one hetero-atom selected from the group consisting of N, O, and S. In some embodiments,  $R^B$  is selected from the group consisting of benzene, pyridine, furan, thiophene.

In some embodiments,  $R^C$  is an aryl ring or a heteroaryl ring comprising one or two nitrogen atoms. In some embodiments,  $R^C$  is selected from the group consisting of benzene, pyridine, imidazole.

In some embodiments, (a) at least one  $R^1$ ,  $R^2$ , or  $R^3$  comprises a substituent selected from the group consisting of carbazole, azacarbazole, dibenzofuran, azadibenzofuran, dibenzothiophene, azadibenzothiophene, dibenzoselenophene, azadibenzoselenophene, triphenylene, azatriphenylene, diphenyl(silyl), triphenyl(silyl), and tetraphenyl(silyl); (b) two adjacent substituents of  $R^1$ ,  $R^2$ , or  $R^3$  form a fused benzo substituent on  $R^A$ ,  $R^B$ , or  $R^C$ , respectively; or (c) both option (a) and option (b) are true.

In some embodiments, at least one  $R^1$ ,  $R^2$ , or  $R^3$  comprises a substituent selected from the group consisting of carbazole, azacarbazole, dibenzofuran, azadibenzofuran, dibenzothiophene, azadibenzothiophene, dibenzoselenophene, azadibenzoselenophene, triphenylene, azatriphenylene, diphenyl(silyl), triphenyl(silyl), and tetraphenyl(silyl); and the remaining substituents  $R^1$ ,  $R^2$ , and  $R^3$  are H. In some embodiments, exactly one  $R^1$ ,  $R^2$ , or  $R^3$  comprises a substituent selected from the group consisting of carbazole, azacarbazole, dibenzofuran, azadibenzofuran, dibenzothiophene, azadibenzothiophene, dibenzoselenophene, azadibenzoselenophene, triphenylene, azatriphenylene, diphenyl(silyl), triphenyl(silyl), and tetraphenyl(silyl); and the remaining substituents  $R^1$ ,  $R^2$ , and  $R^3$  are H.

In some embodiments, exactly one  $R^1$  comprises a substituent selected from the group consisting of carbazole, azacarbazole, dibenzofuran, azadibenzofuran, dibenzothiophene, azadibenzothiophene, dibenzoselenophene, azadibenzoselenophene, triphenylene, azatriphenylene, diphenyl(silyl), triphenyl(silyl), and tetraphenyl(silyl); and the remaining substituents  $R^1$ ,  $R^2$ , and  $R^3$  are H. In some embodiments, exactly one  $R^2$  comprises a substituent selected from the group consisting of carbazole, azacarbazole, dibenzofuran, azadibenzofuran, dibenzothiophene, azadibenzothiophene, dibenzoselenophene, azadibenzoselenophene, triphenylene, azatriphenylene, diphenyl(silyl), triphenyl(silyl), and tetraphenyl(silyl); and the remaining substituents  $R^1$ ,  $R^2$ , and  $R^3$  are H. In some embodiments, exactly one  $R^3$  comprises a substituent selected from the group consisting of carbazole, azacarbazole, dibenzofuran, azadibenzofuran, dibenzothiophene, azadibenzothiophene,

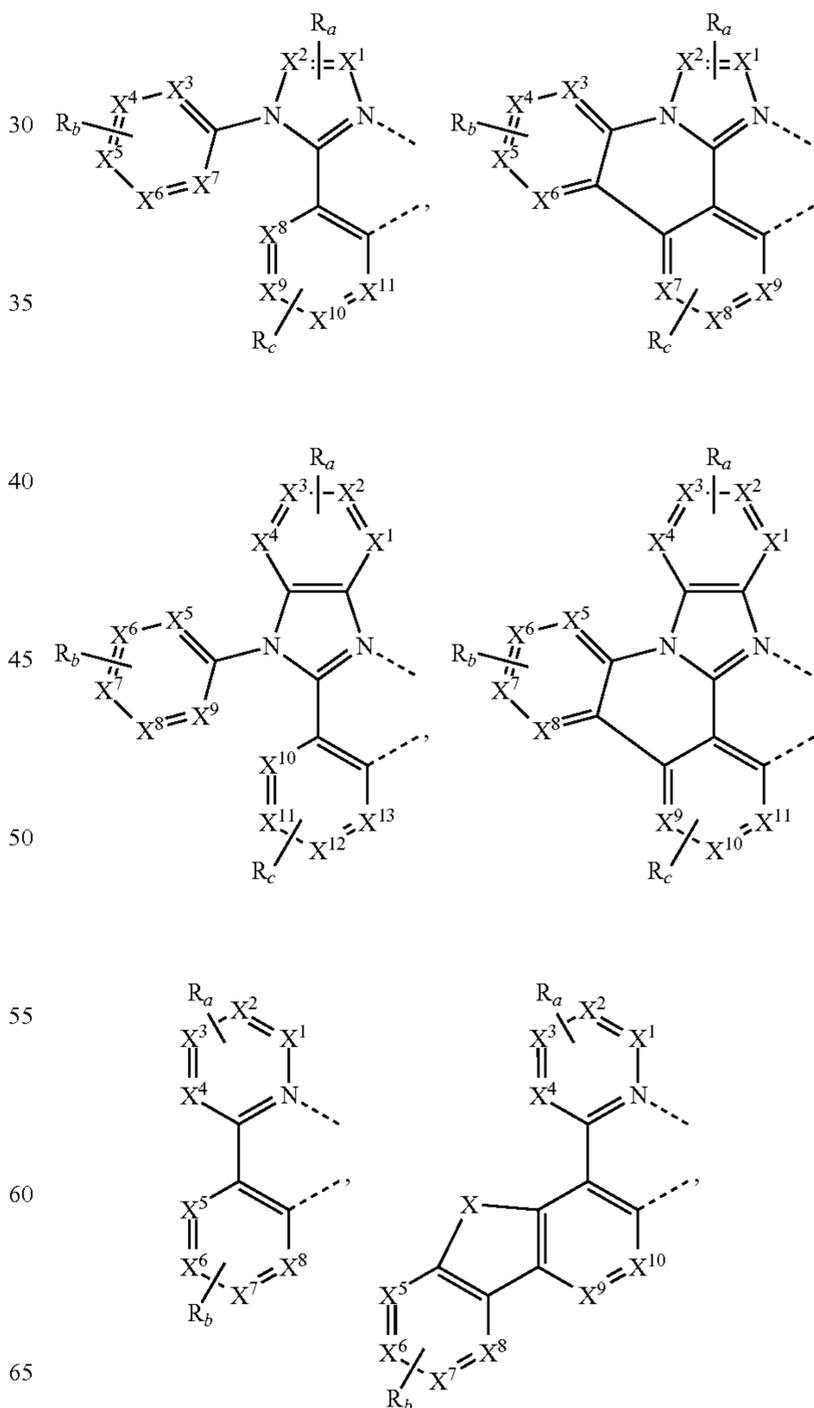
60

dibenzoselenophene, azadibenzoselenophene, triphenylene, azatriphenylene, diphenyl(silyl), triphenyl(silyl), and tetraphenyl(silyl); and the remaining substituents  $R^1$ ,  $R^2$ , and  $R^3$  are H.

According to another embodiment, an OLED is described. The OLED includes an anode; a cathode; and an organic layer, disposed between the anode and the cathode. In such embodiments, the organic layer includes a compound having a structure of Formula I, and its variations described herein. In some embodiments, the organic layer is an emissive layer and the compound is a host.

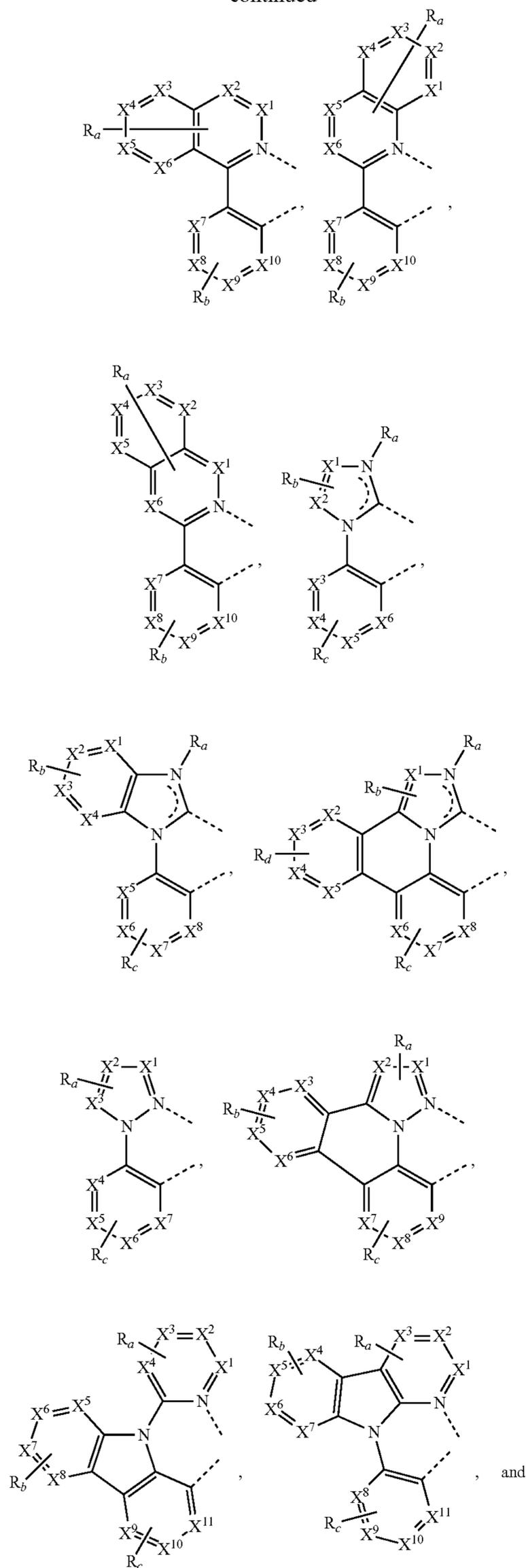
In some embodiments, the OLED is incorporated into a device selected from the group consisting of a consumer product, an electronic component module, and a lighting panel.

In some embodiments, the organic layer further comprises an emissive dopant. The emissive dopant can be a phosphorescent dopant and/or a fluorescent dopant. In some such embodiments, the emissive dopant is a transition metal complex having at least one ligand or part of the ligand, if the ligand is more than bidentate, selected from the group consisting of:



61

-continued



62

-continued

5

10

In the emissive dopant ligand structure:

15 each  $X^1$  to  $X^{13}$  is independently selected from the group consisting of carbon and nitrogen;

$X$  is selected from the group consisting of  $BR'$ ,  $NR'$ ,  $PR'$ ,  $O$ ,  $S$ ,  $Se$ ,  $C=O$ ,  $S=O$ ,  $SO_2$ ,  $CR'R''$ ,  $SiR'R''$ , and  $GeR'R''$ ;

$R'$  and  $R''$  are optionally fused or joined to form a ring;

20 each  $R_a$ ,  $R_b$ ,  $R_c$ , and  $R_d$  may represent from mono substitution to the possible maximum number of substitutions, or no substitution;

$R'$ ,  $R''$ ,  $R_a$ ,  $R_b$ ,  $R_c$ , and  $R_d$  are each independently selected

25 from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and

30 combinations thereof; and any two adjacent substituents of  $R_a$ ,  $R_b$ ,  $R_c$ , and  $R_d$  are optionally fused or joined to form a ring or form a multi-

dentate ligand.

In some embodiments, the organic layer is a charge carrier

35 blocking layer and the compound is a charge carrier blocking material in the organic layer. In some embodiments, the organic layer is an charge carrier transporting layer and the compound is a charge carrier transporting material in the

organic layer.

40 In another embodiment, a formulation comprising a compound having a structure of Formula I and its variations described herein is disclosed. The formulation can include one or more components selected from the group consisting

45 of a solvent, a host, a hole injection material, hole transport material, and an electron transport layer material, disclosed herein.

Combination with Other Materials

The materials described herein as useful for a particular

50 layer in an organic light emitting device may be used in combination with a wide variety of other materials present in the device. For example, emissive dopants disclosed herein may be used in conjunction with a wide variety of

55 hosts, transport layers, blocking layers, injection layers, electrodes and other layers that may be present. The materials described or referred to below are non-limiting examples of materials that may be useful in combination

with the compounds disclosed herein, and one of skill in the art can readily consult the literature to identify other materials that may be useful in combination.

60 Conductivity Dopants:

A charge transport layer can be doped with conductivity

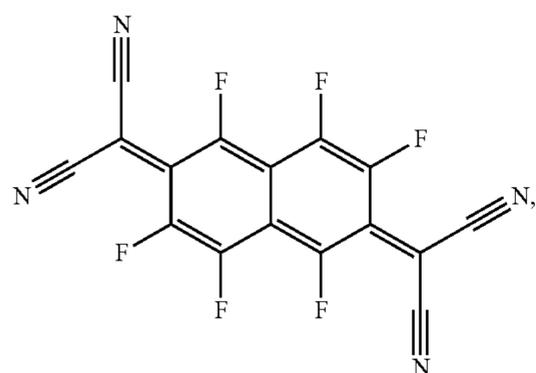
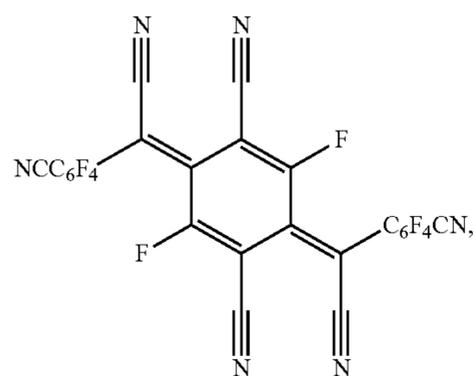
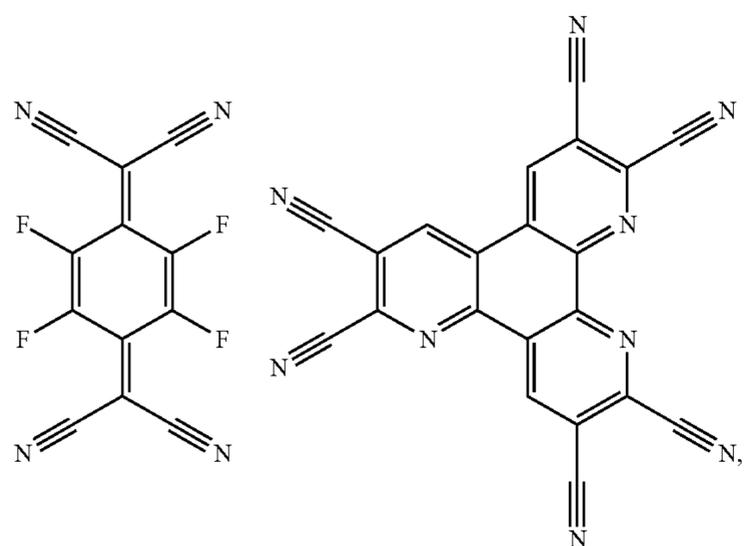
dopants to substantially alter its density of charge carriers, which will in turn alter its conductivity. The conductivity is

65 increased by generating charge carriers in the matrix material, and depending on the type of dopant, a change in the Fermi level of the semiconductor may also be achieved.

63

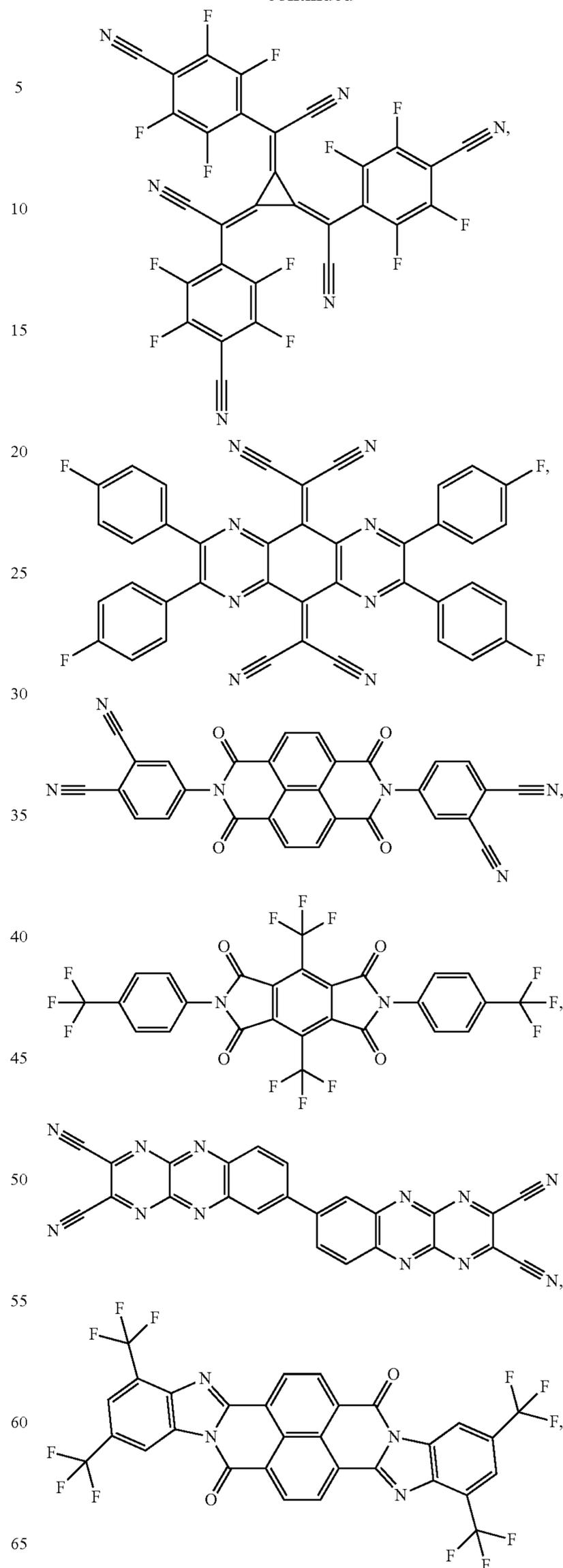
Hole-transporting layer can be doped by p-type conductivity dopants and n-type conductivity dopants are used in the electron-transporting layer.

Non-limiting examples of the conductivity dopants that may be used in an OLED in combination with materials disclosed herein are exemplified below together with references that disclose those materials: EP01617493, EP01968131, EP2020694, EP2684932, US20050139810, US20070160905, US20090167167, US2010288362, WO06081780, WO2009003455, WO2009008277, WO2009011327, WO2014009310, US2007252140, US2015060804 and US2012146012.

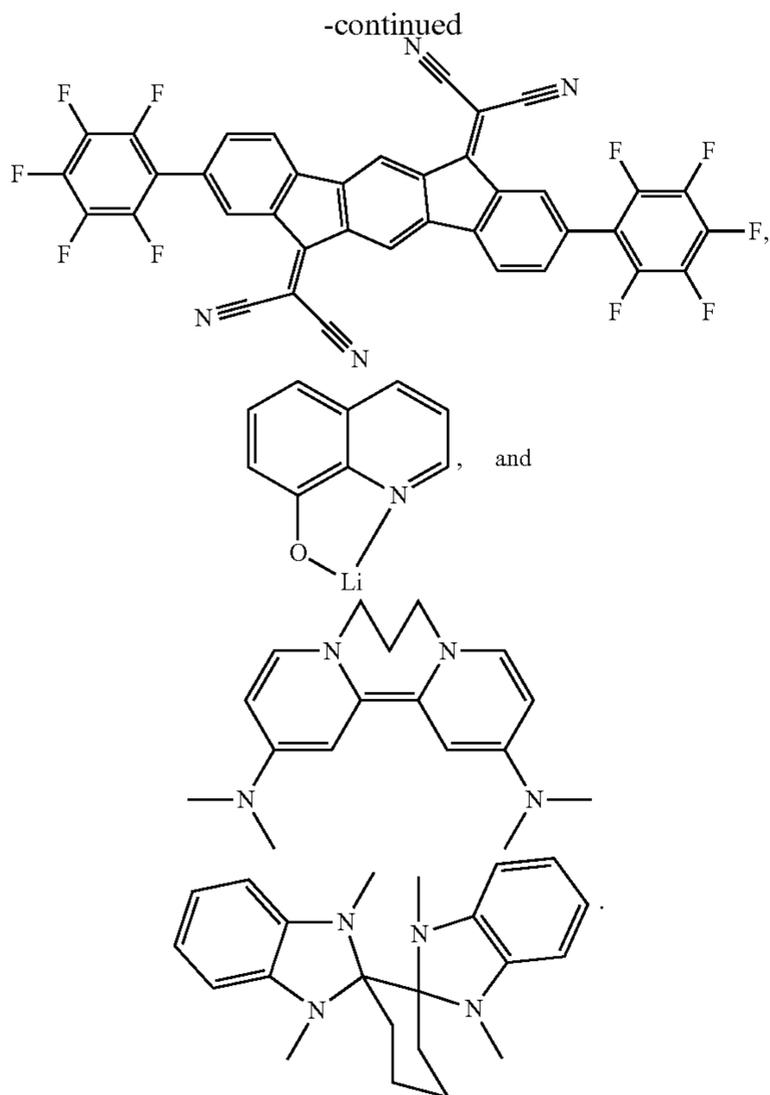


64

-continued



65



5

10

15

20

25

30

35

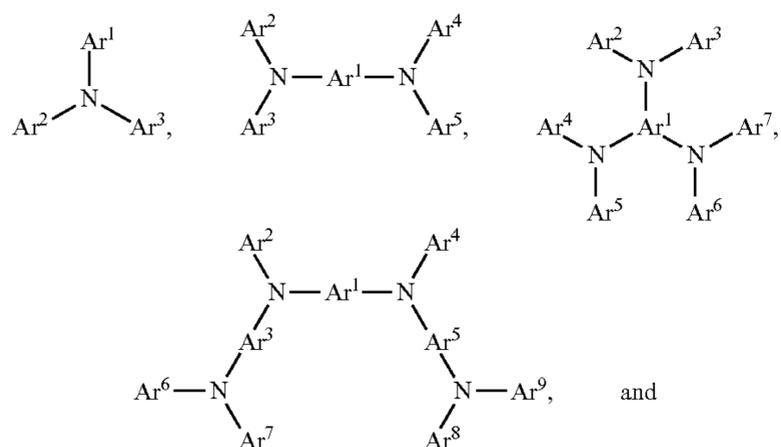
40

45

## HIL/HTL:

A hole injecting/transporting material to be used in the present invention is not particularly limited, and any compound may be used as long as the compound is typically used as a hole injecting/transporting material. Examples of the material include, but are not limited to: a phthalocyanine or porphyrin derivative; an aromatic amine derivative; an indolocarbazole derivative; a polymer containing fluorohydrocarbon; a polymer with conductivity dopants; a conducting polymer, such as PEDOT/PSS; a self-assembly monomer derived from compounds such as phosphonic acid and silane derivatives; a metal oxide derivative, such as  $\text{MoO}_x$ ; a p-type semiconducting organic compound, such as 1,4,5,8,9,12-Hexaazatriphenylenehexacarbonitrile; a metal complex, and a cross-linkable compounds.

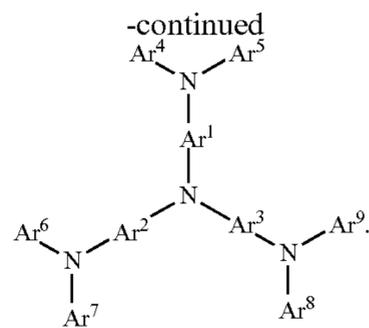
Examples of aromatic amine derivatives used in HIL or HTL include, but are not limited to the following general structures:



60

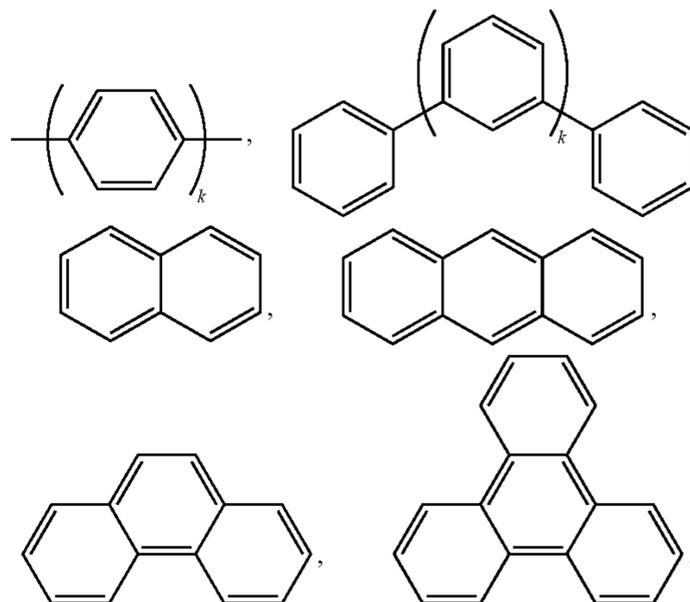
65

66



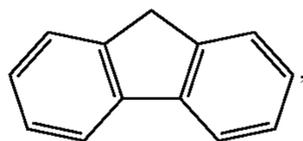
Each of  $\text{Ar}^1$  to  $\text{Ar}^9$  is selected from the group consisting of aromatic hydrocarbon cyclic compounds such as benzene, biphenyl, triphenyl, triphenylene, naphthalene, anthracene, phenalene, phenanthrene, fluorene, pyrene, chrysene, perylene, and azulene; the group consisting of aromatic heterocyclic compounds such as dibenzothiophene, dibenzofuran, dibenzoselenophene, furan, thiophene, benzofuran, benzothiophene, benzoselenophene, carbazole, indolocarbazole, pyridylindole, pyrrolodipyridine, pyrazole, imidazole, triazole, oxazole, thiazole, oxadiazole, oxatriazole, dioxazole, thiadiazole, pyridine, pyridazine, pyrimidine, pyrazine, triazine, oxazine, oxathiazine, oxadiazine, indole, benzimidazole, indazole, indoxazine, benzoxazole, benzisoxazole, benzothiazole, quinoline, isoquinoline, cinoline, quinazoline, quinoxaline, naphthyridine, phthalazine, pteridine, xanthene, acridine, phenazine, phenothiazine, phenoxazine, benzofuropyridine, furodipyridine, benzothienopyridine, thienodipyridine, benzoselenophenopyridine, and selenophenodipyridine; and the group consisting of 2 to 10 cyclic structural units which are groups of the same type or different types selected from the aromatic hydrocarbon cyclic group and the aromatic heterocyclic group and are bonded to each other directly or via at least one of oxygen atom, nitrogen atom, sulfur atom, silicon atom, phosphorus atom, boron atom, chain structural unit and the aliphatic cyclic group. Each Ar may be unsubstituted or may be substituted by a substituent selected from the group consisting of deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof.

In one aspect,  $\text{Ar}^1$  to  $\text{Ar}^9$  is independently selected from the group consisting of:

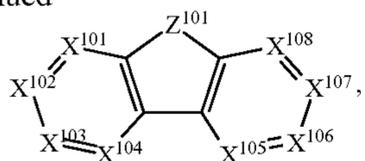


67

-continued

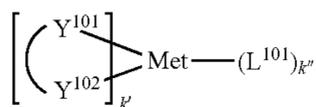


and



wherein  $k$  is an integer from 1 to 20;  $X^{101}$  to  $X^{108}$  is C (including CH) or N;  $Z^{101}$  is  $NAr^1$ , O, or S;  $Ar^1$  has the same group defined above.

Examples of metal complexes used in HIL or HTL include, but are not limited to the following general formula:



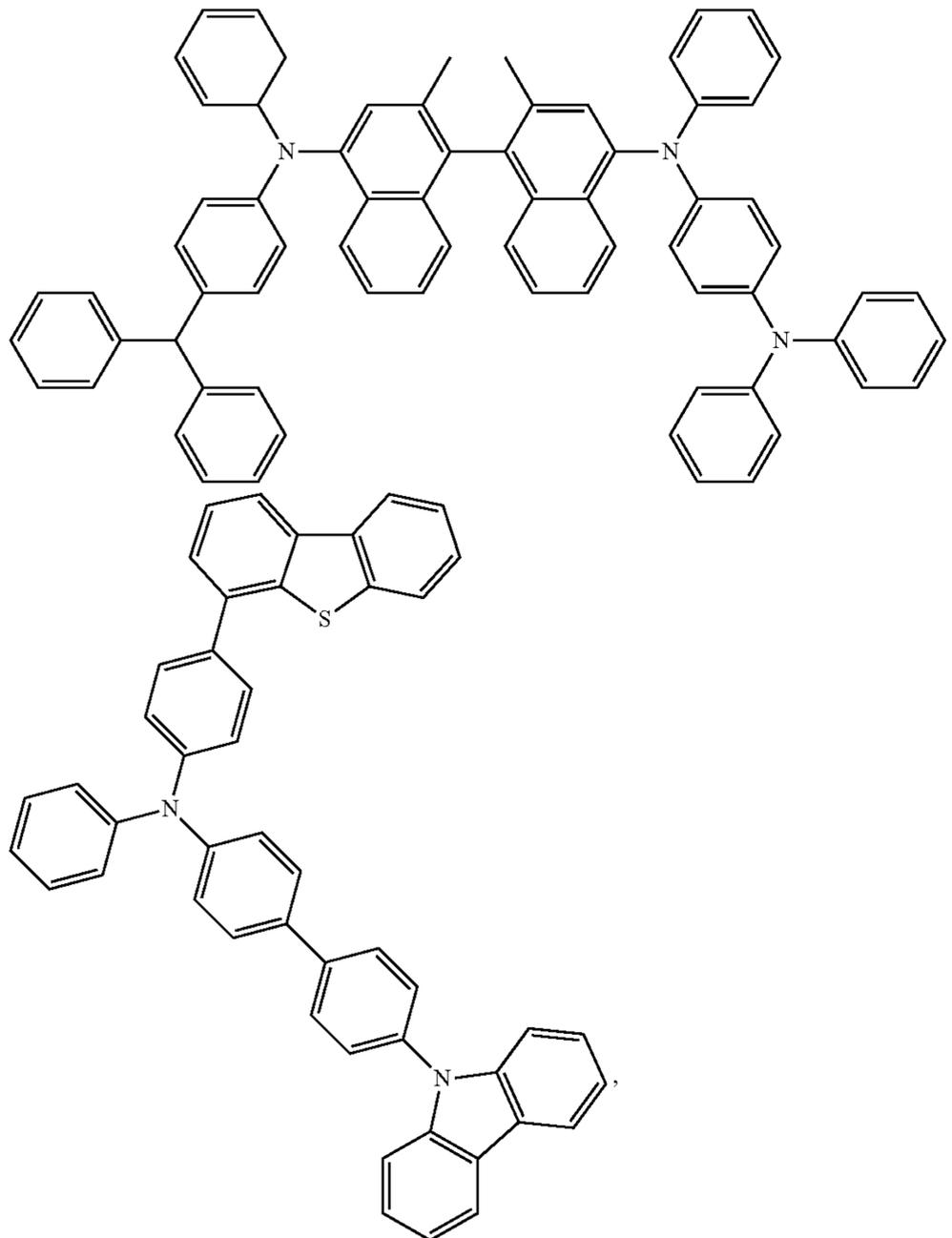
wherein Met is a metal, which can have an atomic weight greater than 40;  $(Y^{101}-Y^{102})$  is a bidentate ligand,  $Y^{101}$  and  $Y^{102}$  are independently selected from C, N, O, P, and S;  $L^{101}$  is an ancillary ligand;  $k'$  is an integer value from 1 to the maximum number of ligands that may be attached to the metal; and  $k'+k''$  is the maximum number of ligands that may be attached to the metal.

In one aspect,  $(Y^{101}-Y^{102})$  is a 2-phenylpyridine derivative. In another aspect,  $(Y^{101}-Y^{102})$  is a carbene ligand. In another aspect, Met is selected from Ir, Pt, Os, and Zn. In a

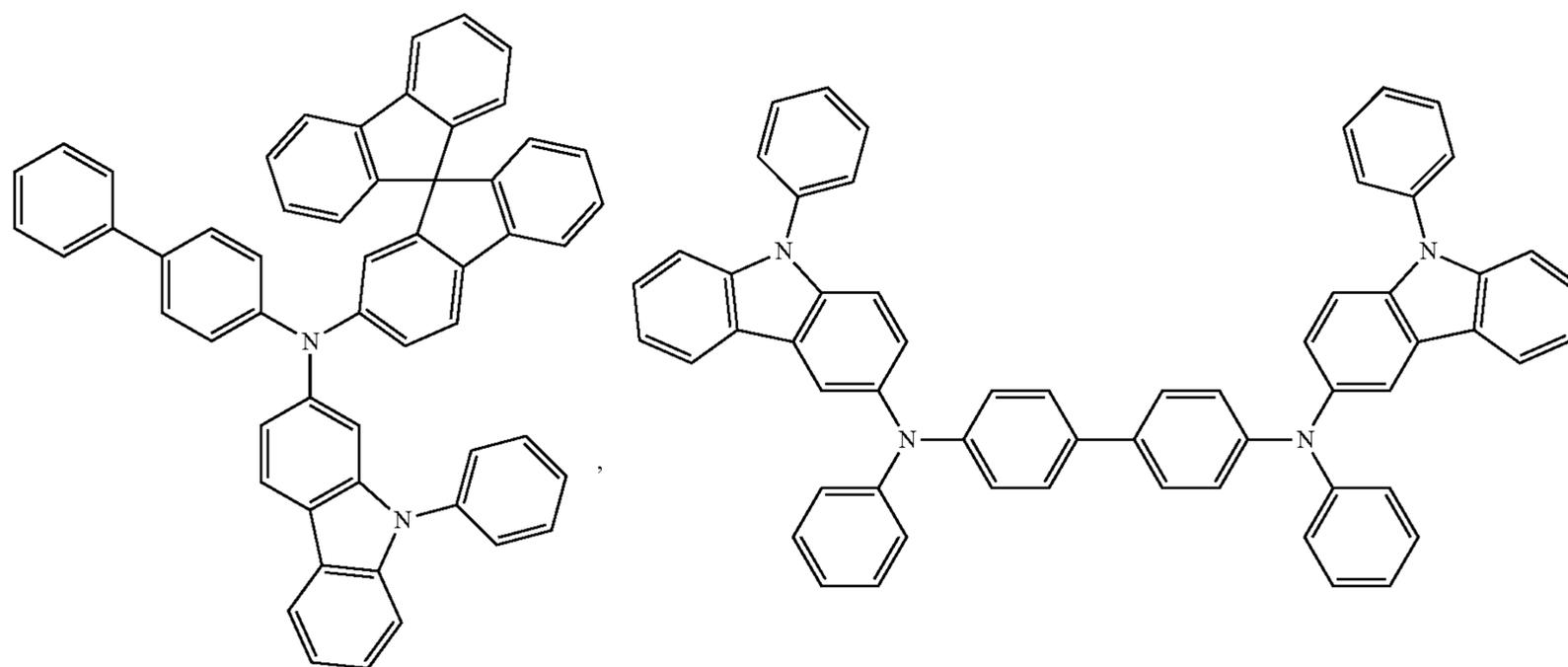
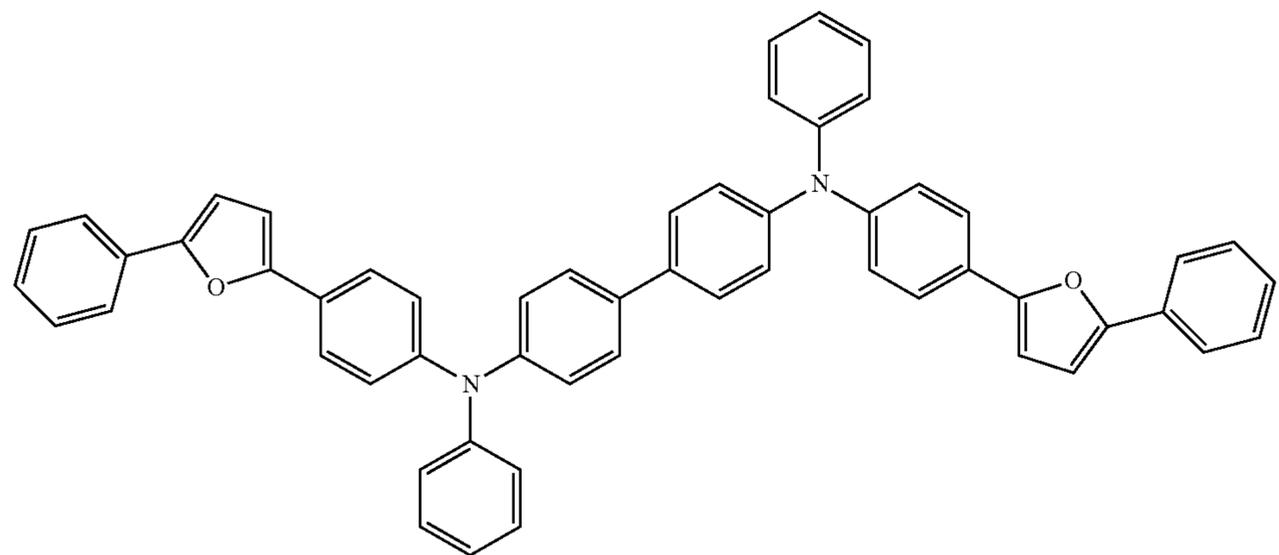
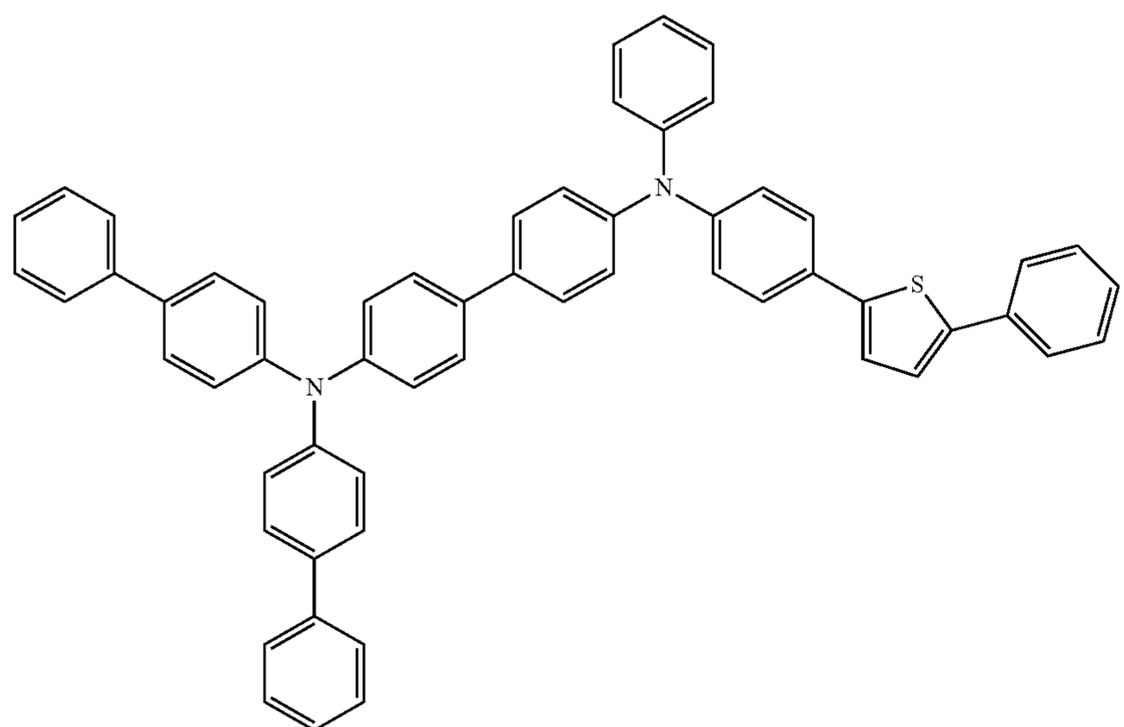
68

further aspect, the metal complex has a smallest oxidation potential in solution vs.  $Fc^+/Fc$  couple less than about 0.6 V.

Non-limiting examples of the HIL and HTL materials that may be used in an OLED in combination with materials disclosed herein are exemplified below together with references that disclose those materials: CN102702075, DE 102012005215, EP01624500, EP01698613, EP01806334, EP01930964, EP01972613, EP01997799, EP02011790, EP02055700, EP02055701, EP1725079, EP2085382, EP2660300, EP650955, JP07-073529, JP2005112765, JP2007091719, JP2008021687, JP2014-009196, KR20110088898, KR20130077473, TW201139402, U.S. Ser. No. 06/517,957, US20020158242, US20030162053, US20050123751, US20060182993, US20060240279, US20070145888, US20070181874, US20070278938, US20080014464, US20080091025, US20080106190, US20080124572, US20080145707, US20080220265, US20080233434, US20080303417, US2008107919, US20090115320, US20090167161, US2009066235, US2011007385, US20110163302, US2011240968, US2011278551, US2012205642, US2013241401, US20140117329, US2014183517, U.S. Pat. Nos. 5,061,569, 5,639,914, WO05075451, WO07125714, WO08023550, WO08023759, WO2009145016, WO2010061824, WO2011075644, WO2012177006, WO2013018530, WO2013039073, WO2013087142, WO2013118812, WO2013120577, WO2013157367, WO2013175747, WO2014002873, WO2014015935, WO2014015937, WO2014030872, WO2014030921, WO2014034791, WO2014104514, WO2014157018.



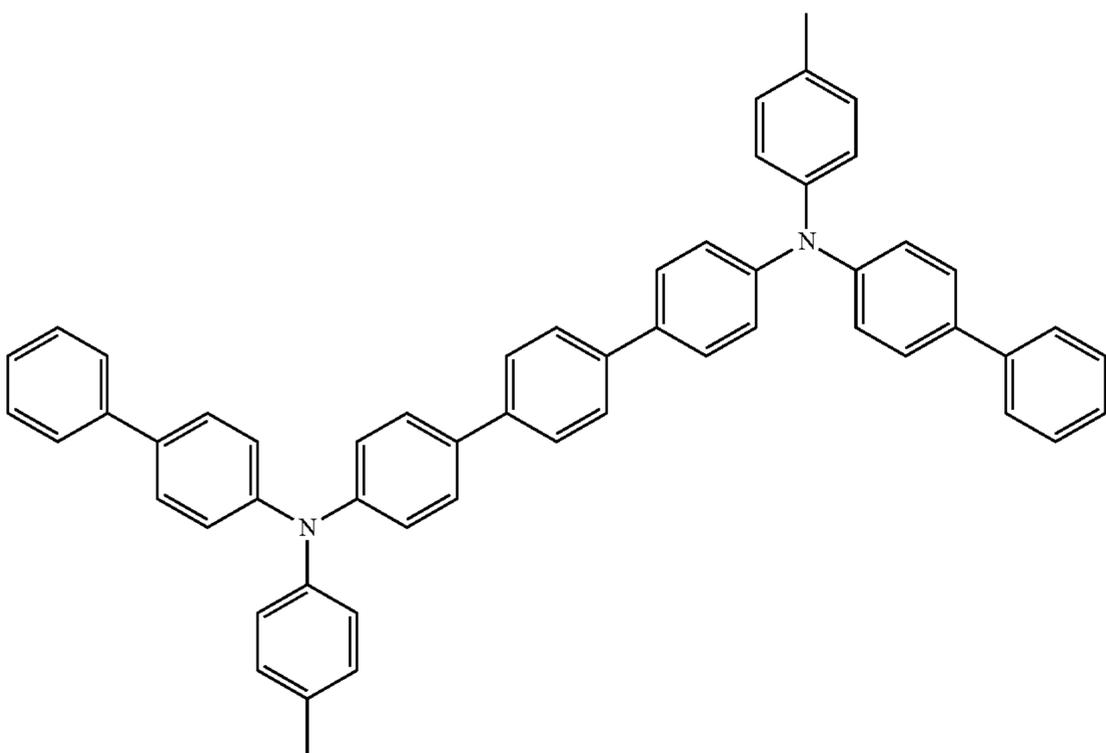
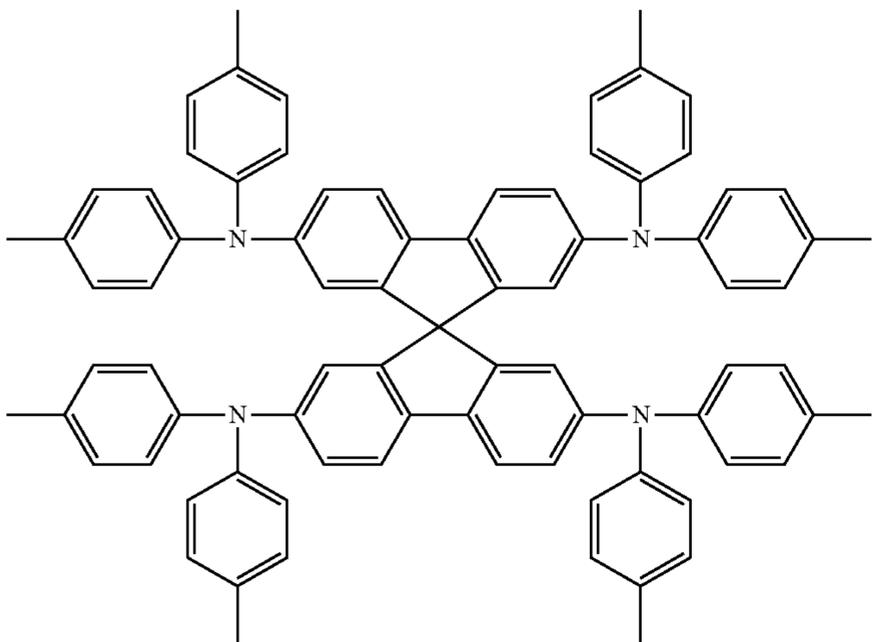
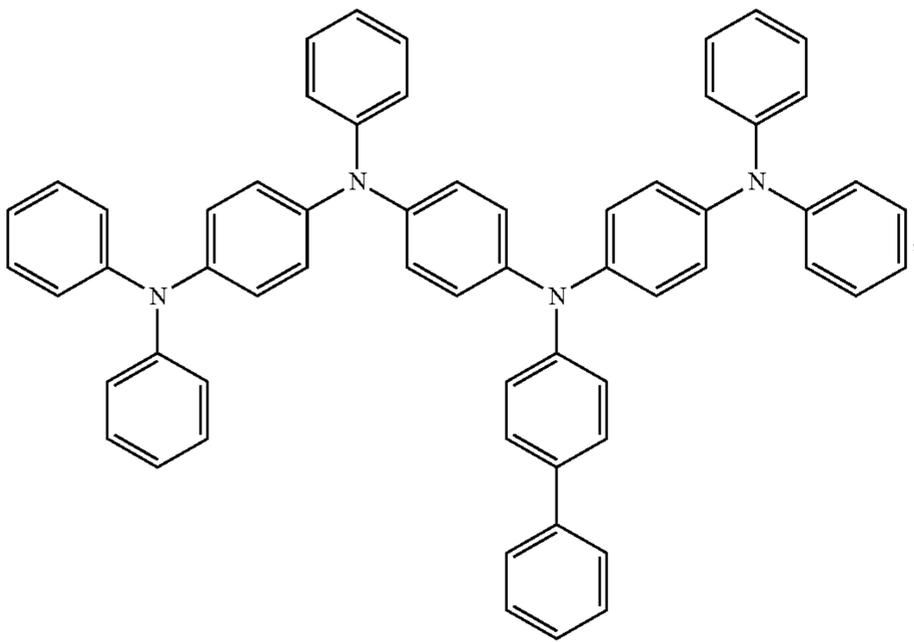
-continued



71

72

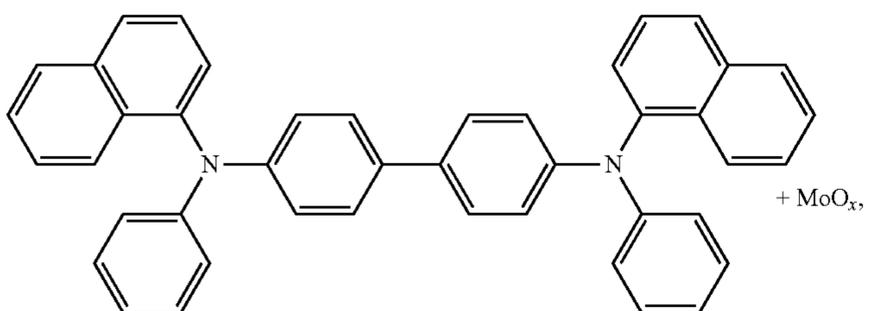
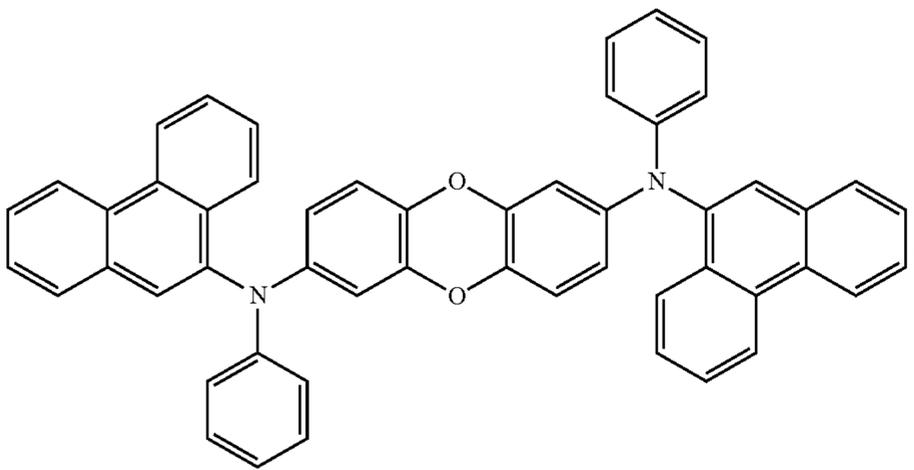
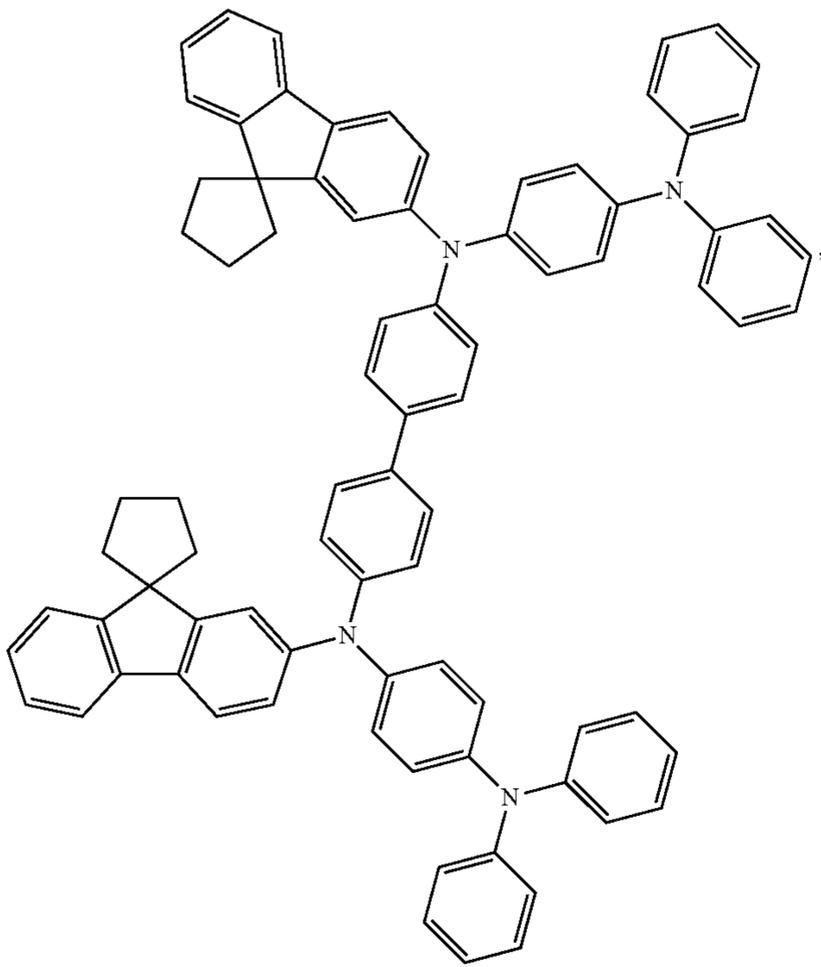
-continued



73

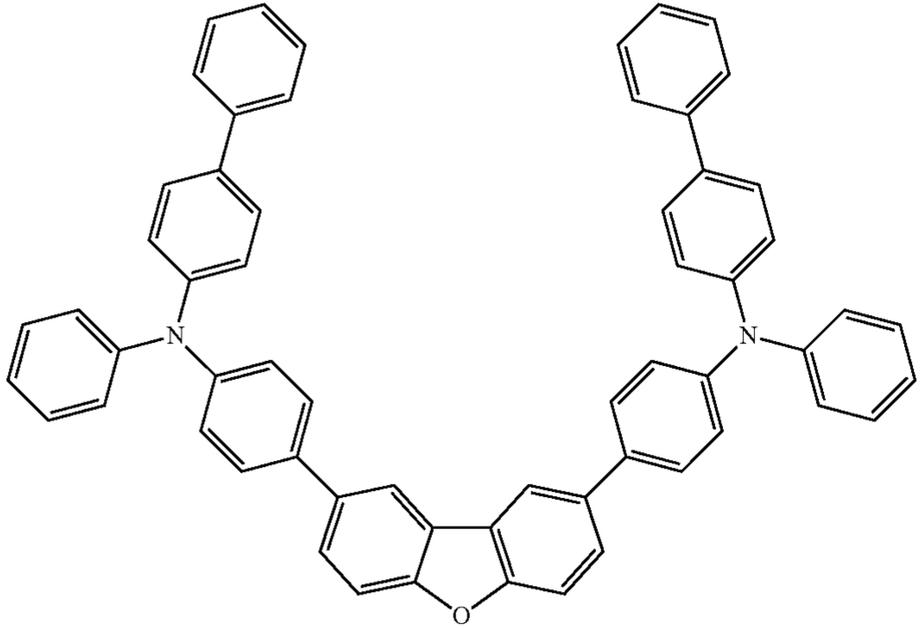
74

-continued

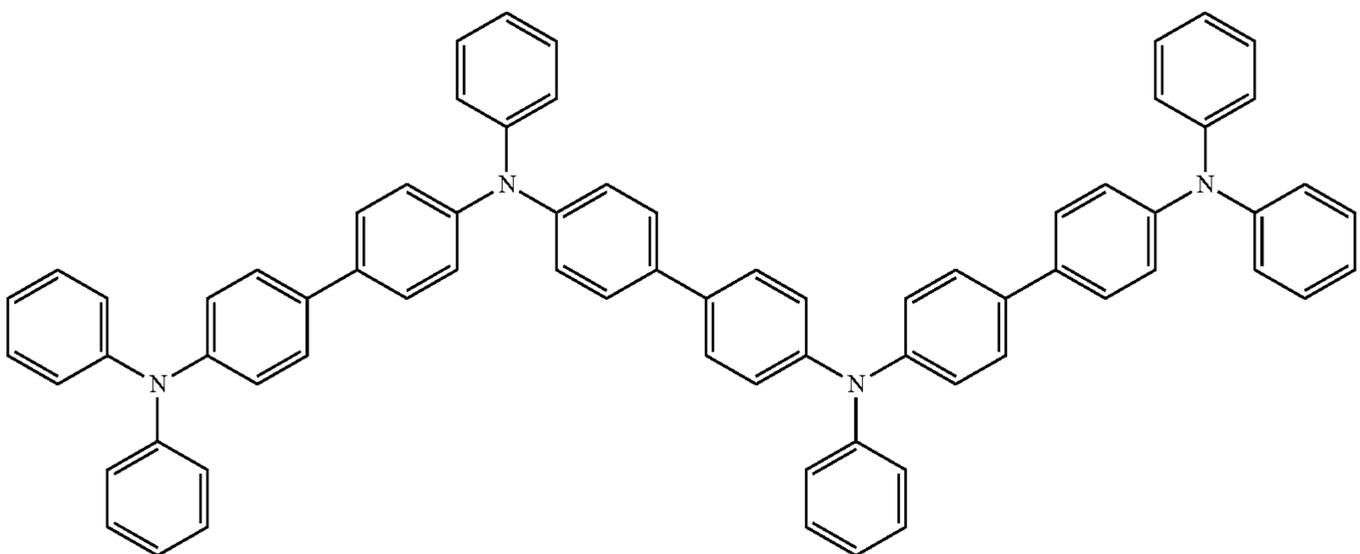
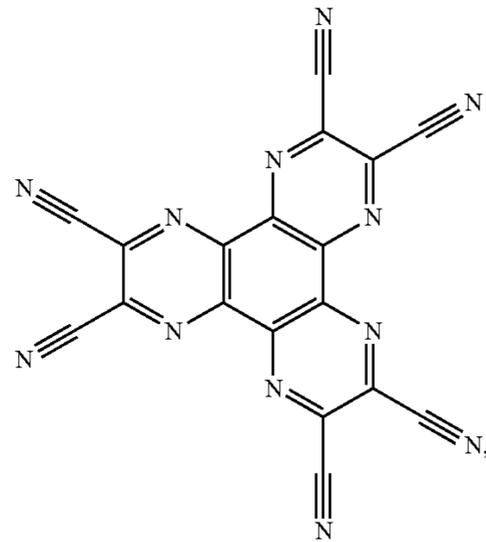
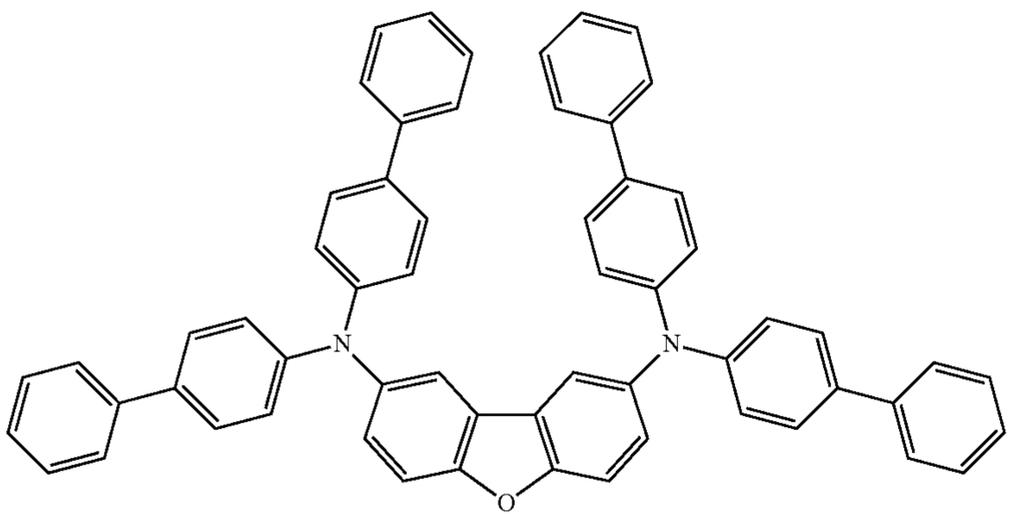
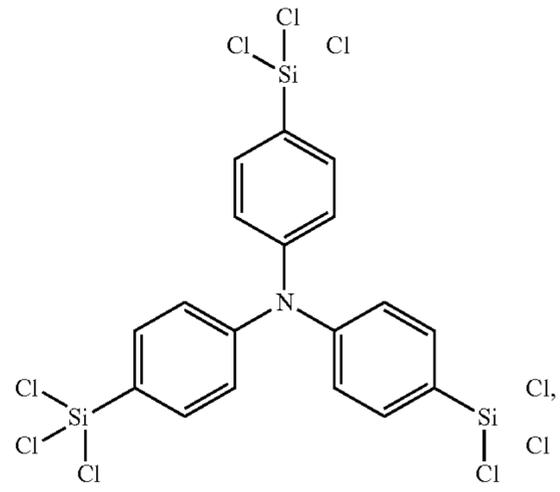


75

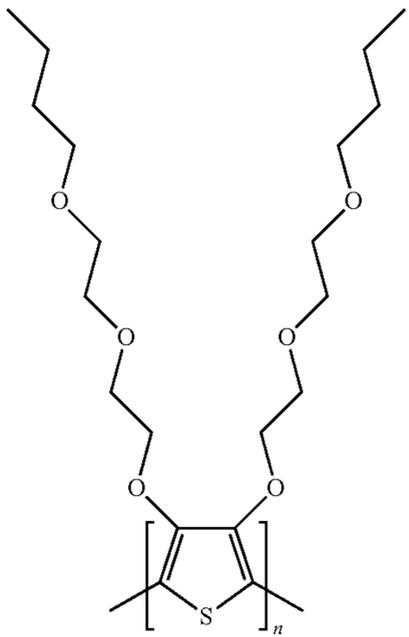
-continued



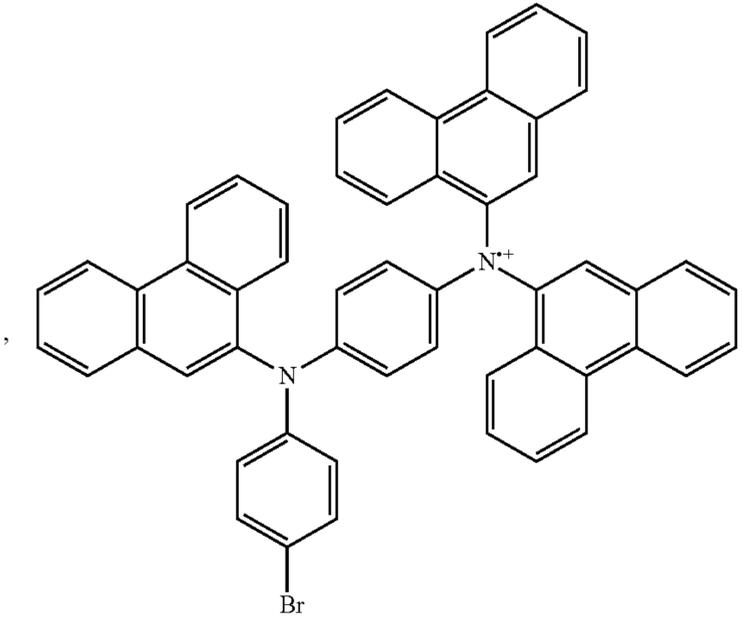
76



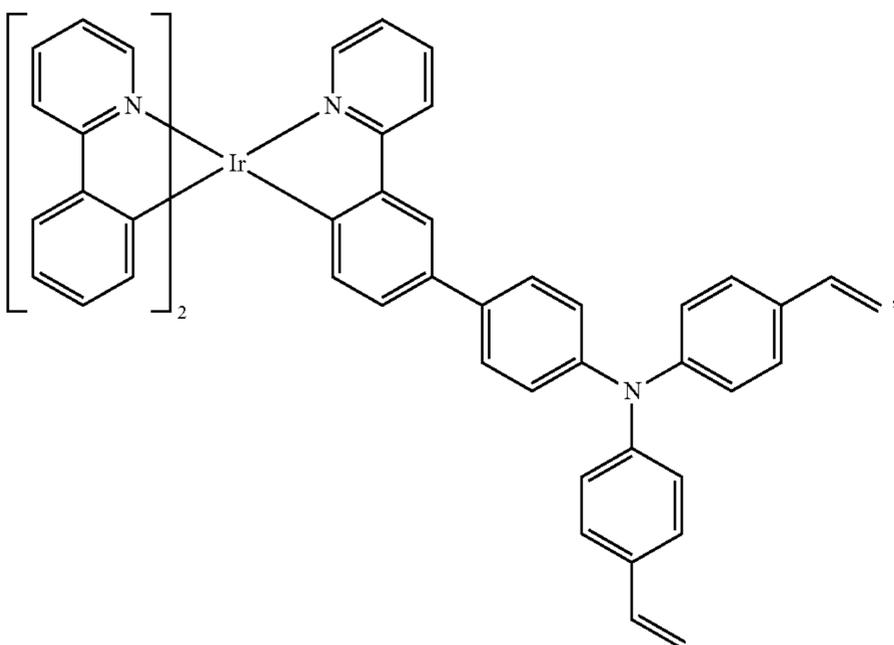
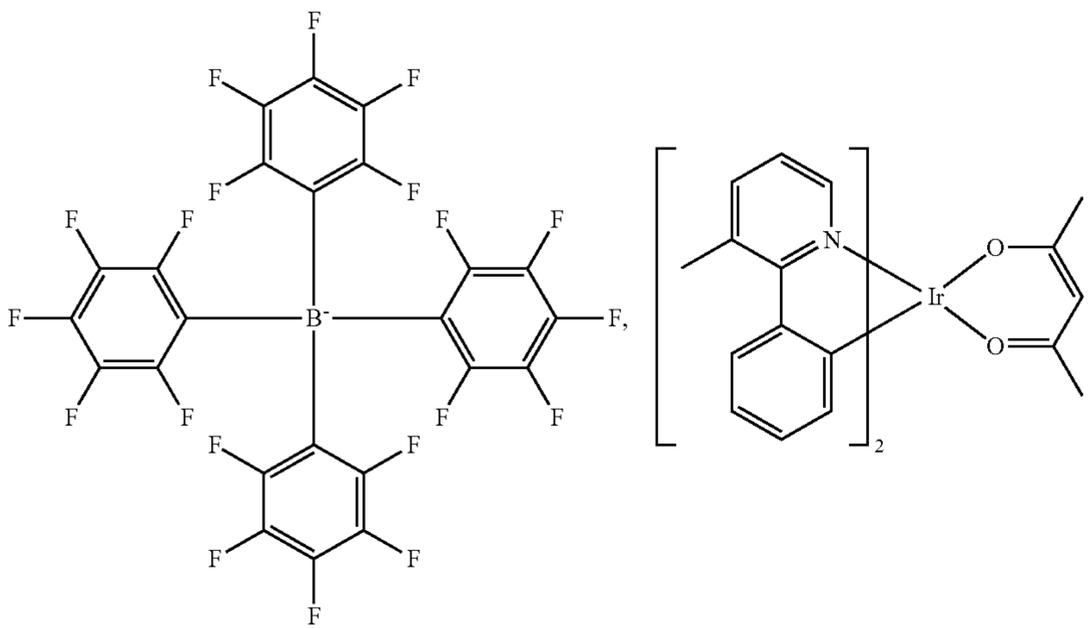
77



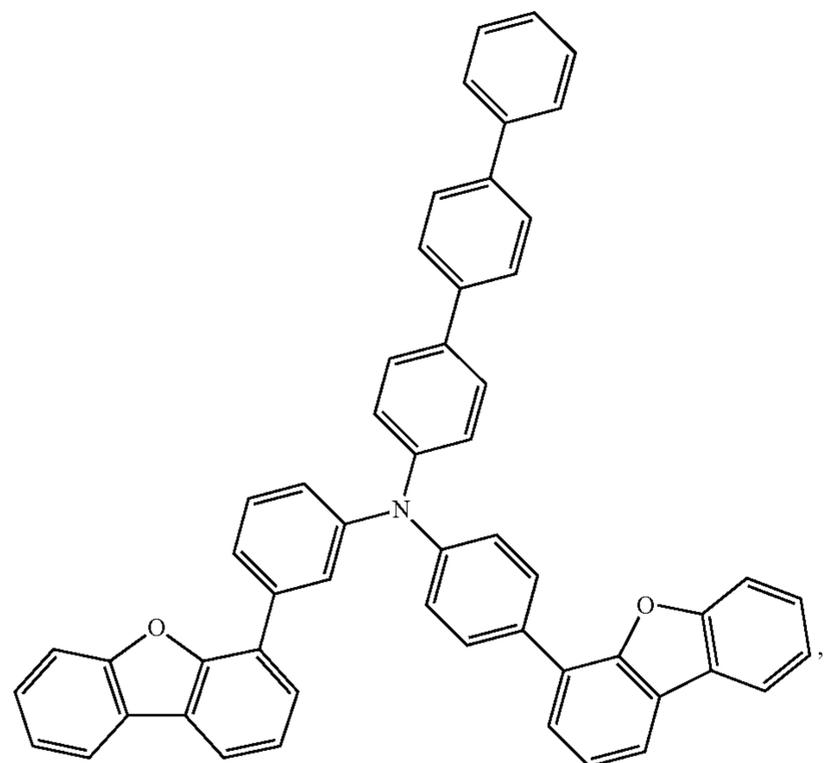
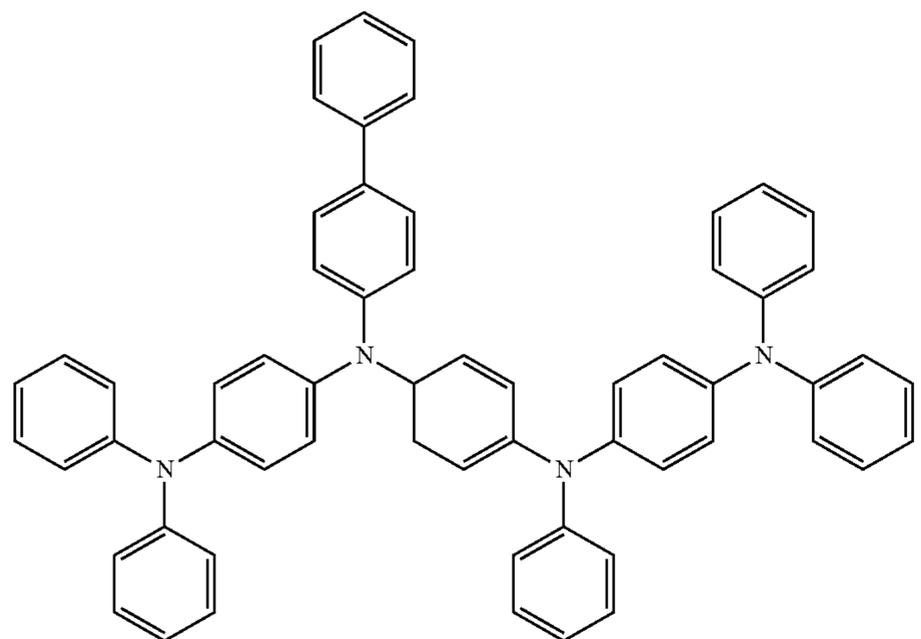
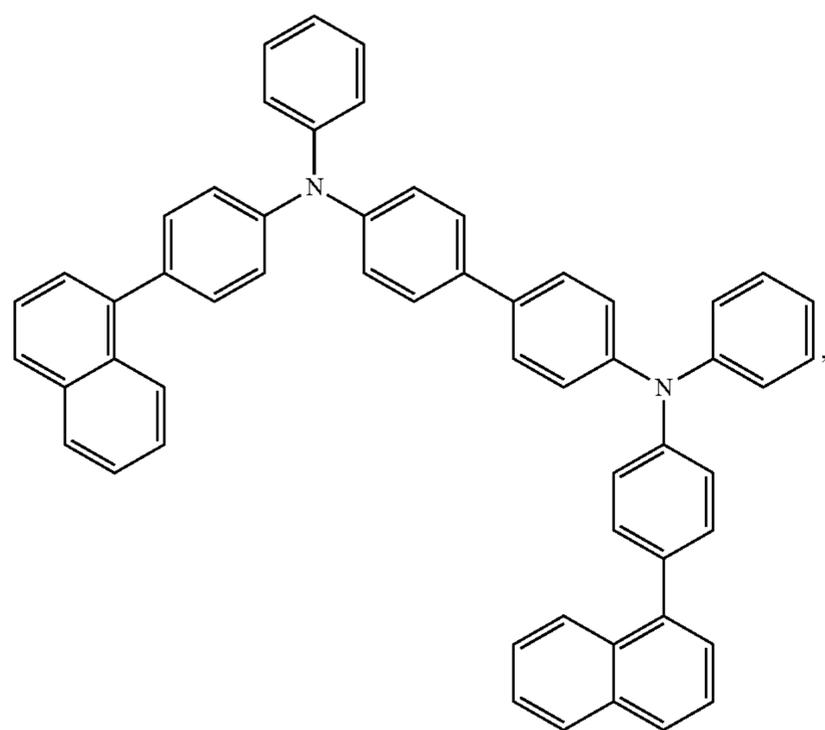
-continued



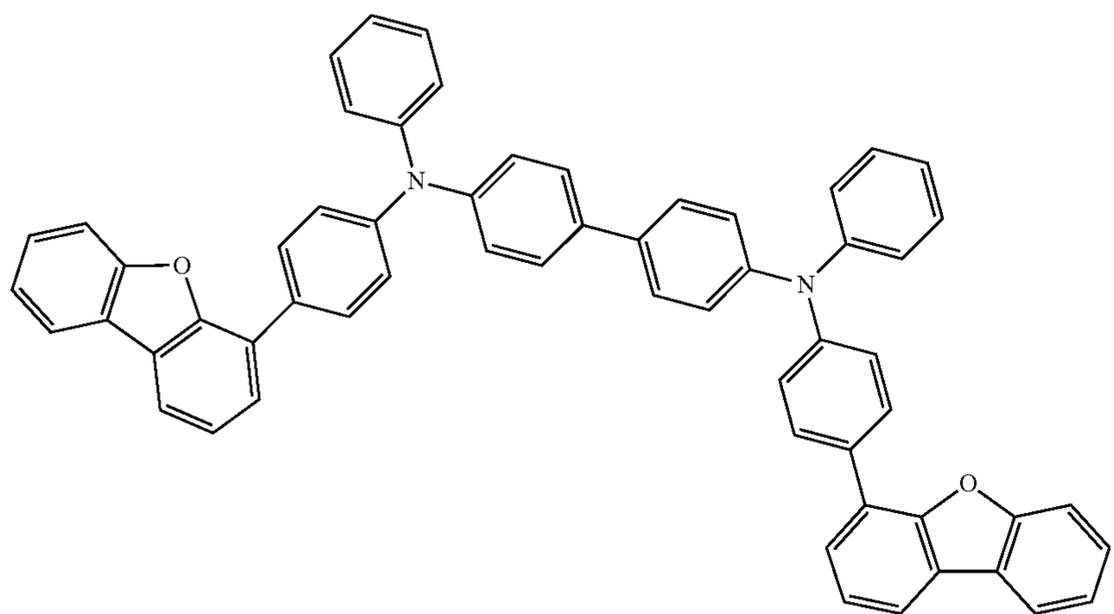
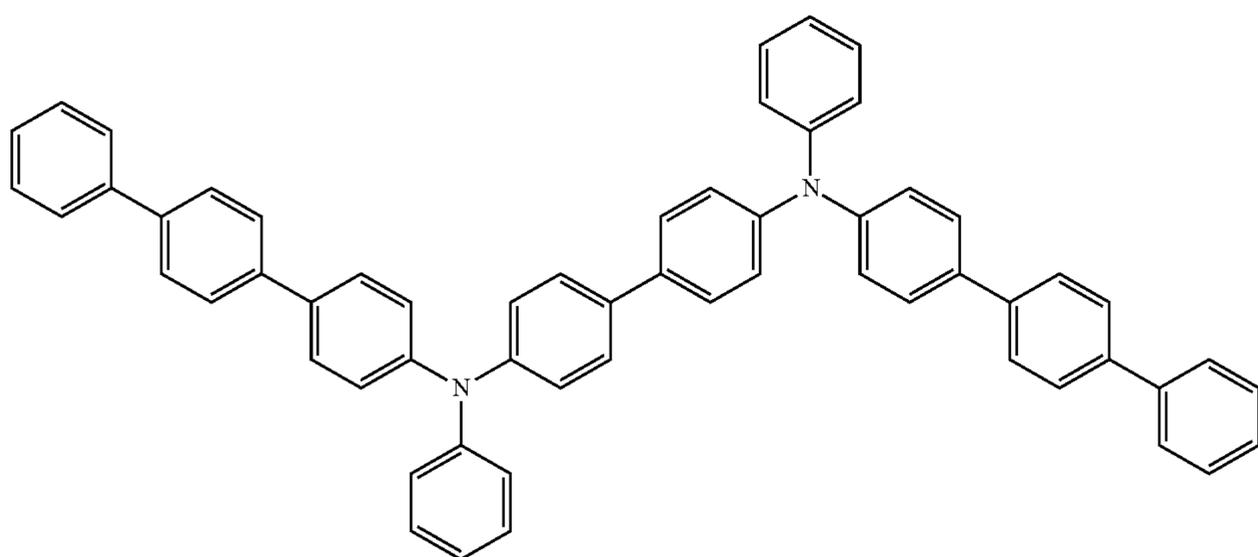
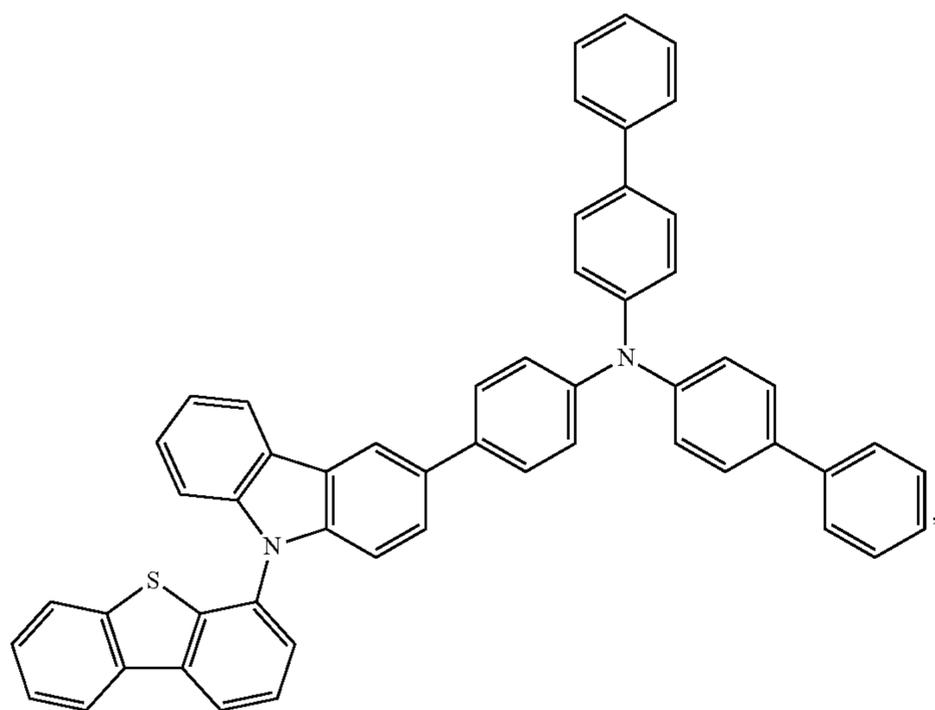
78



-continued



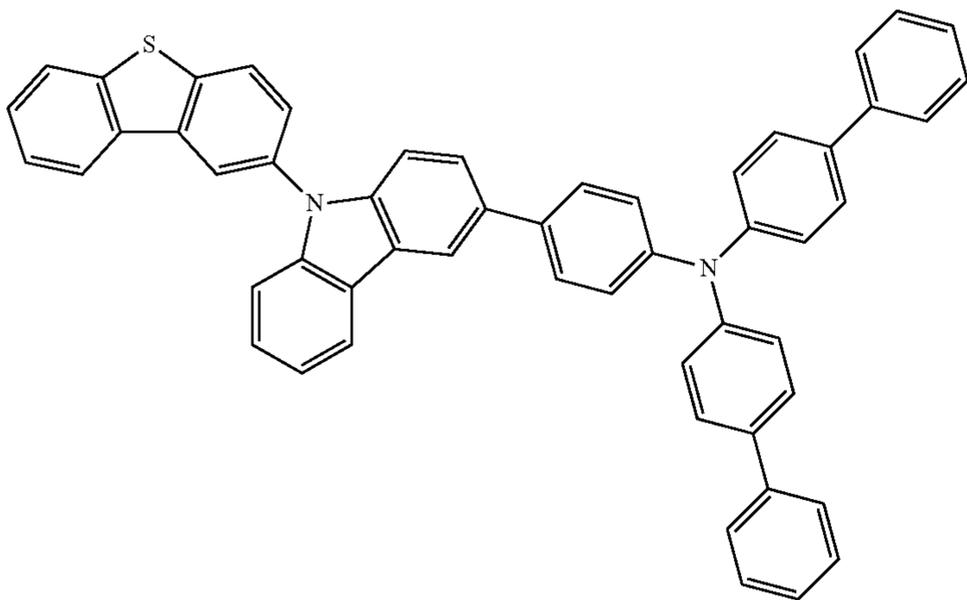
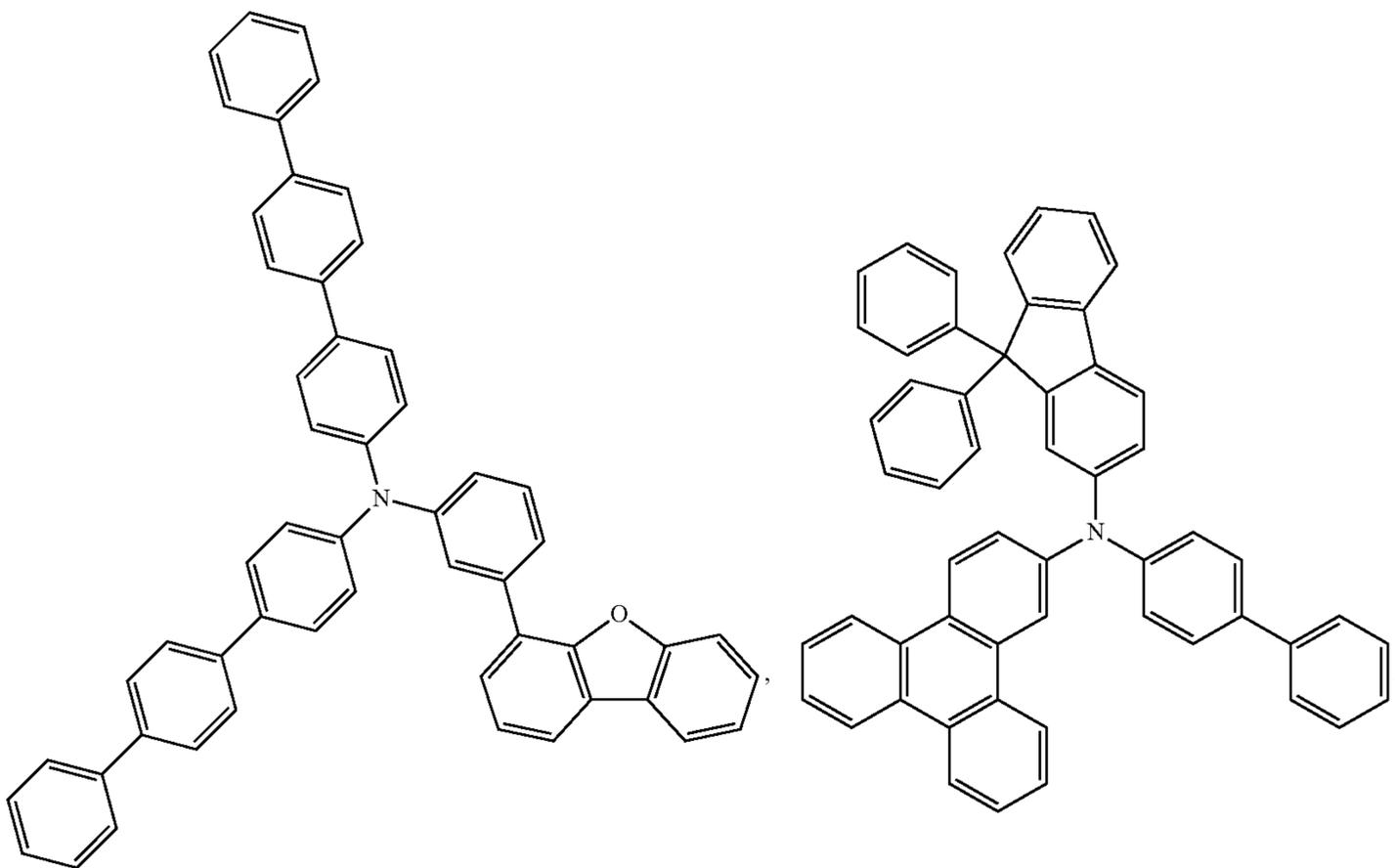
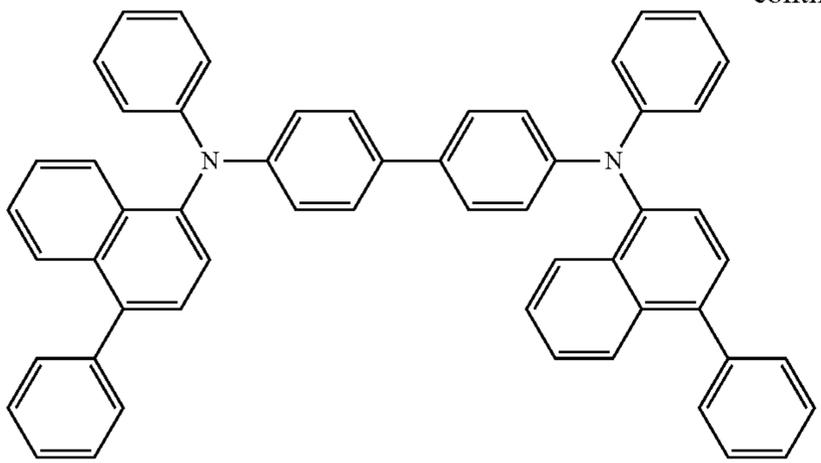
-continued



83

84

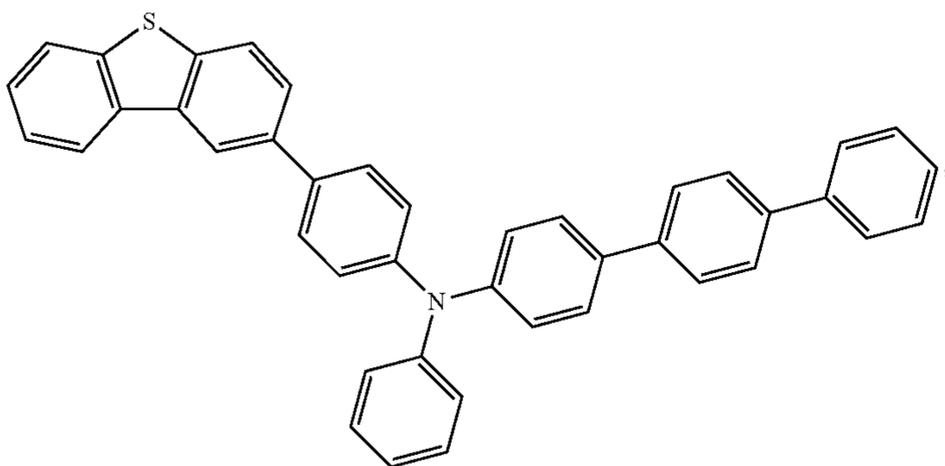
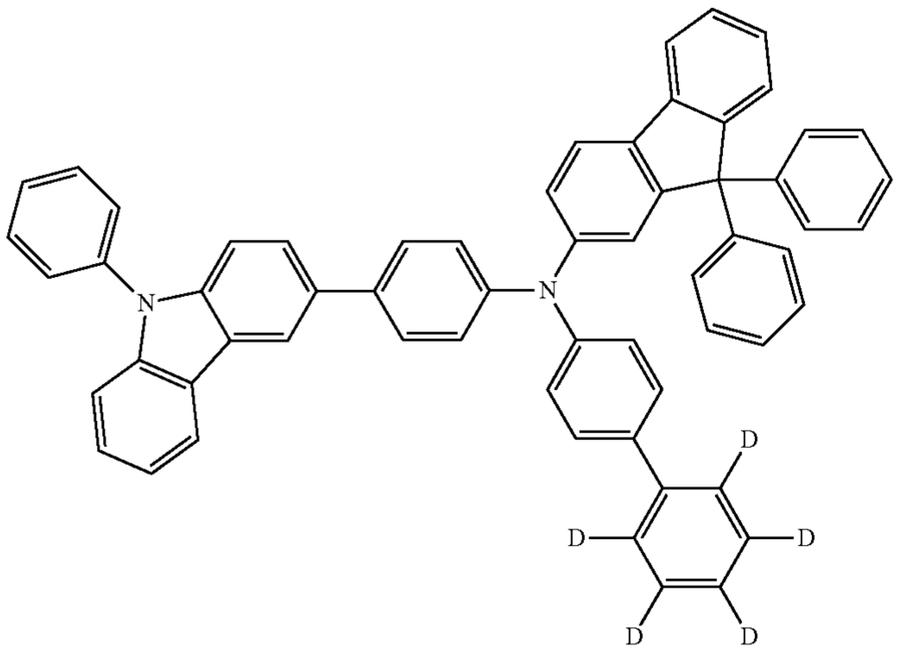
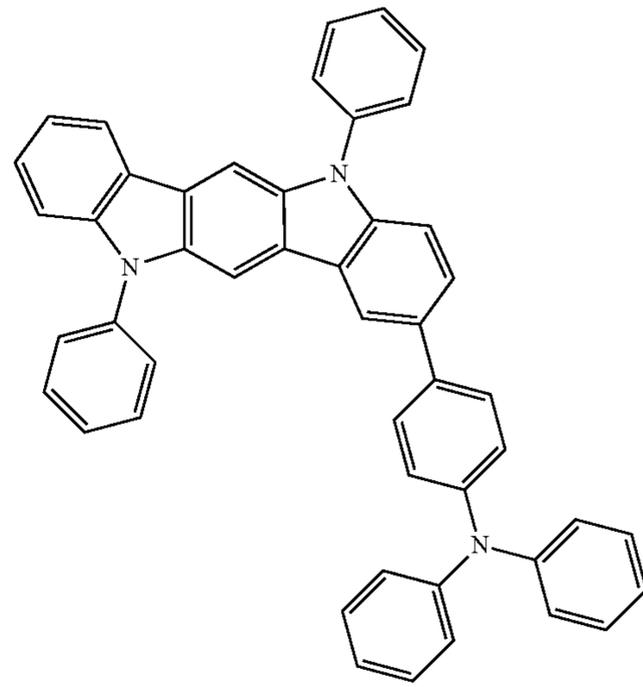
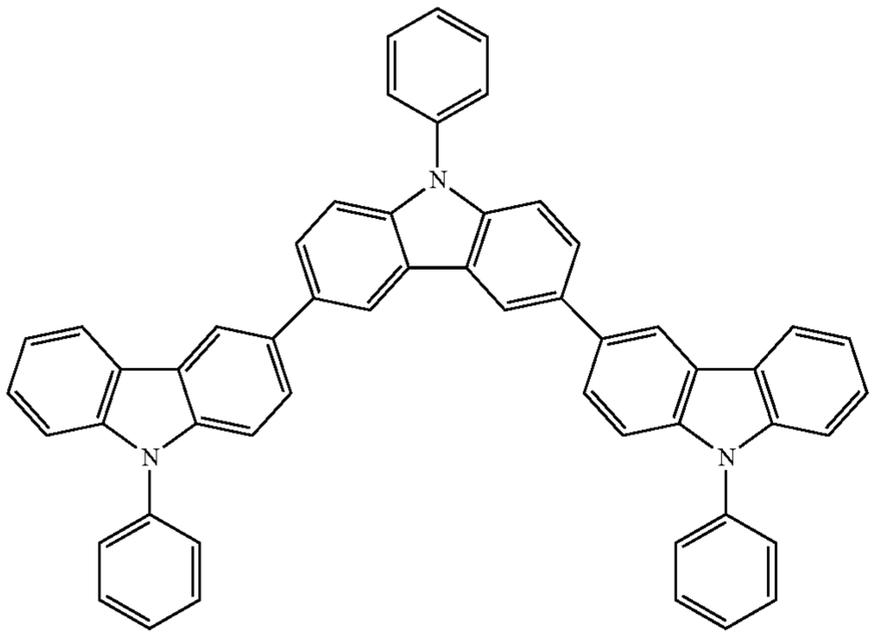
-continued



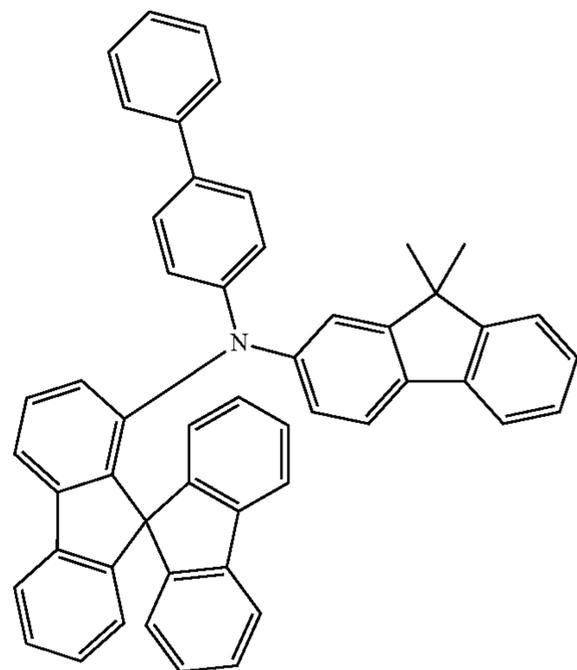
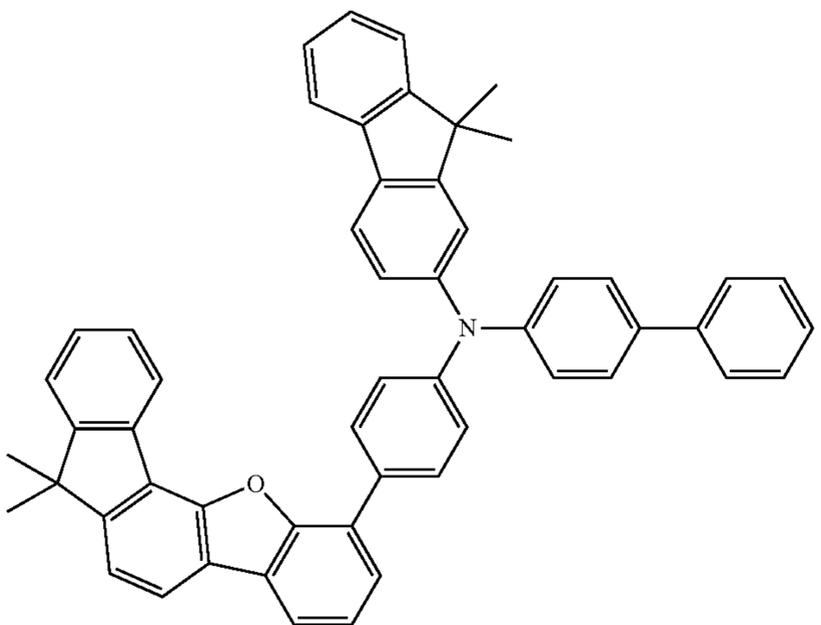
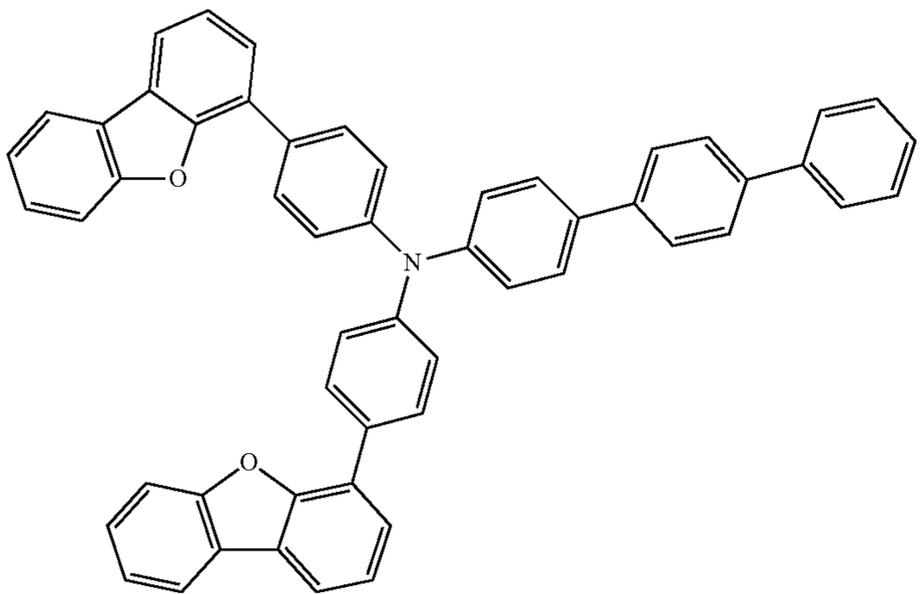
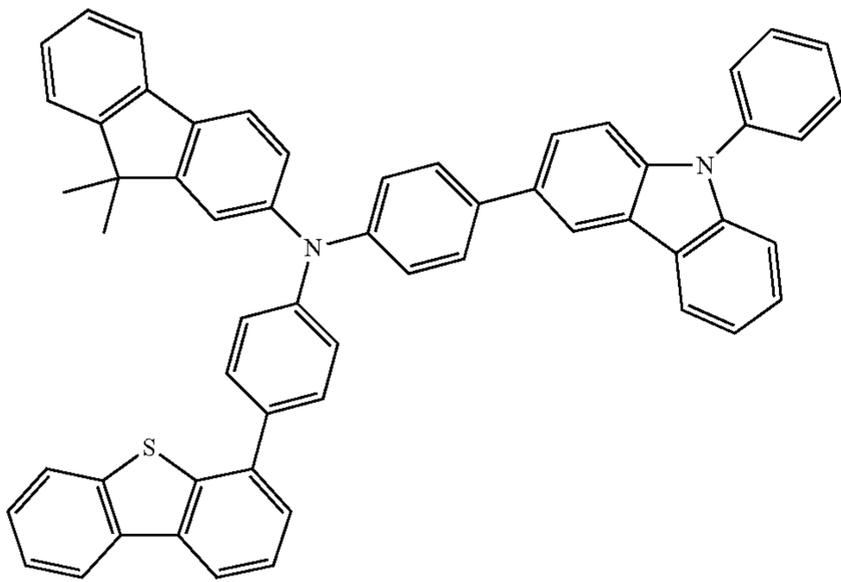
85

-continued

86



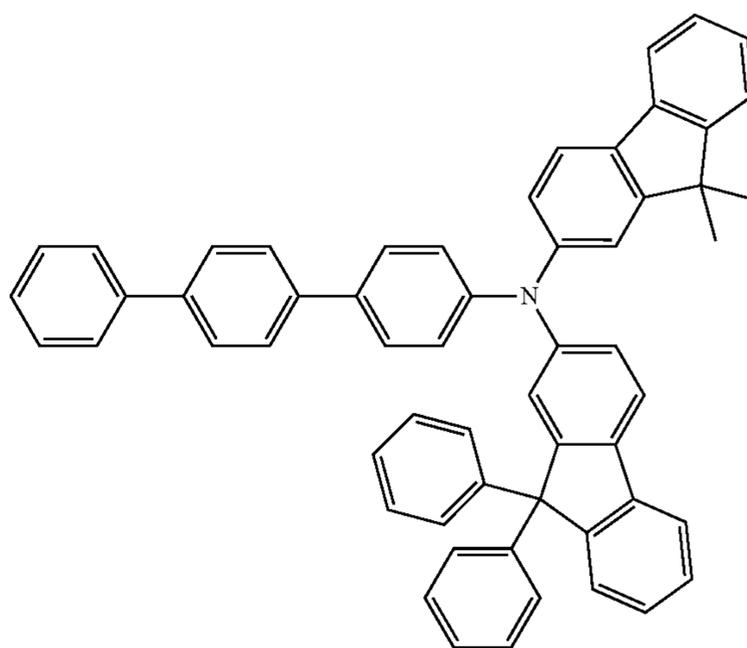
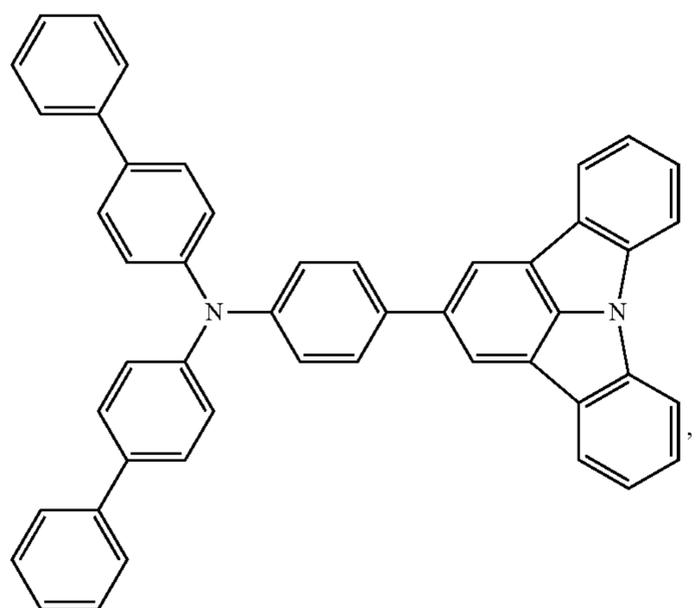
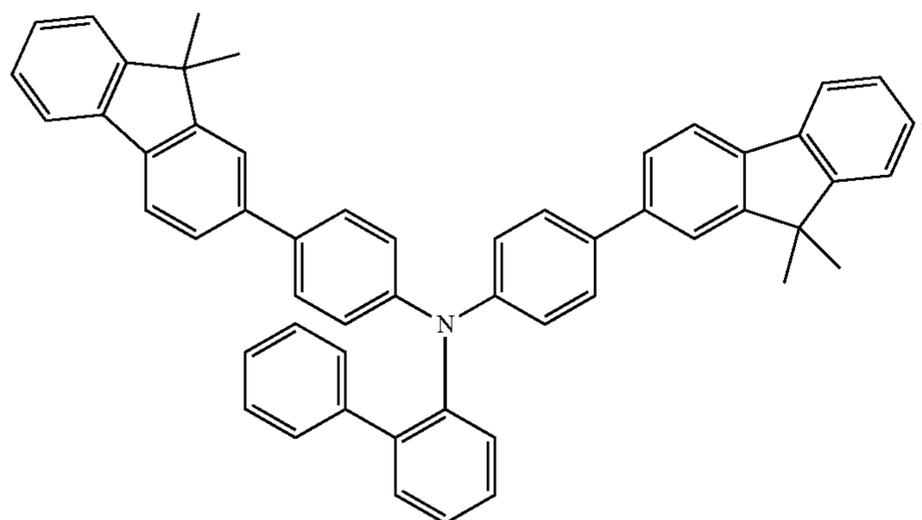
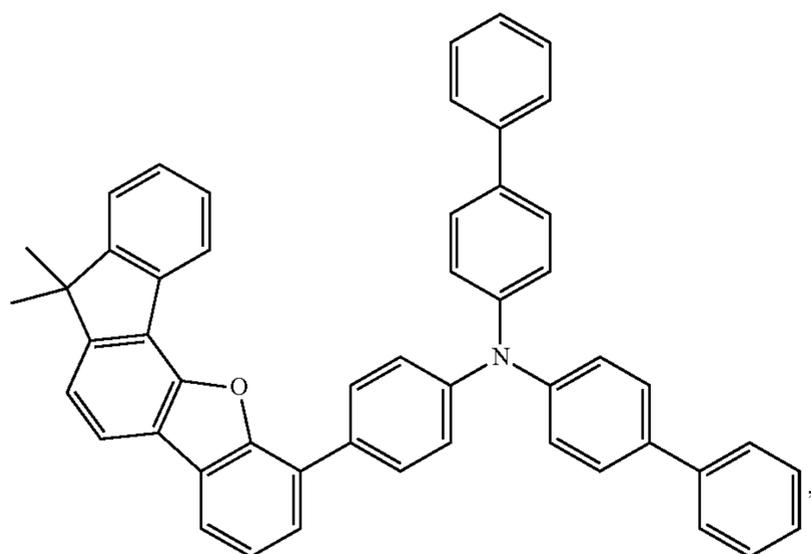
-continued



89

90

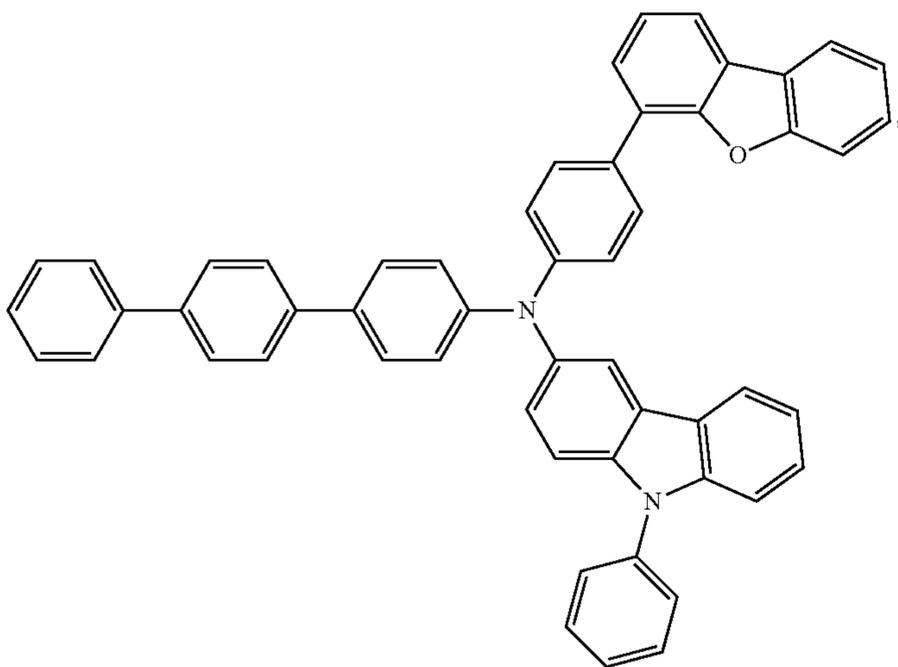
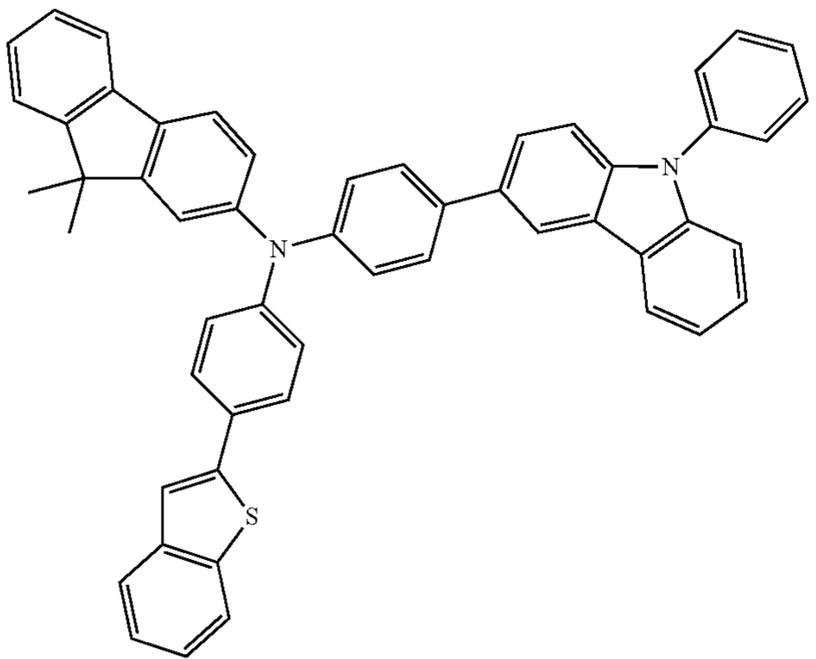
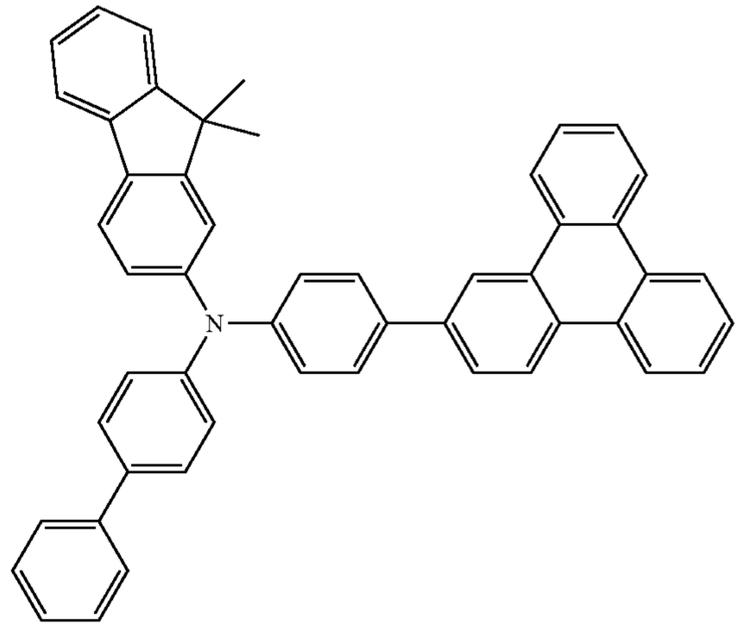
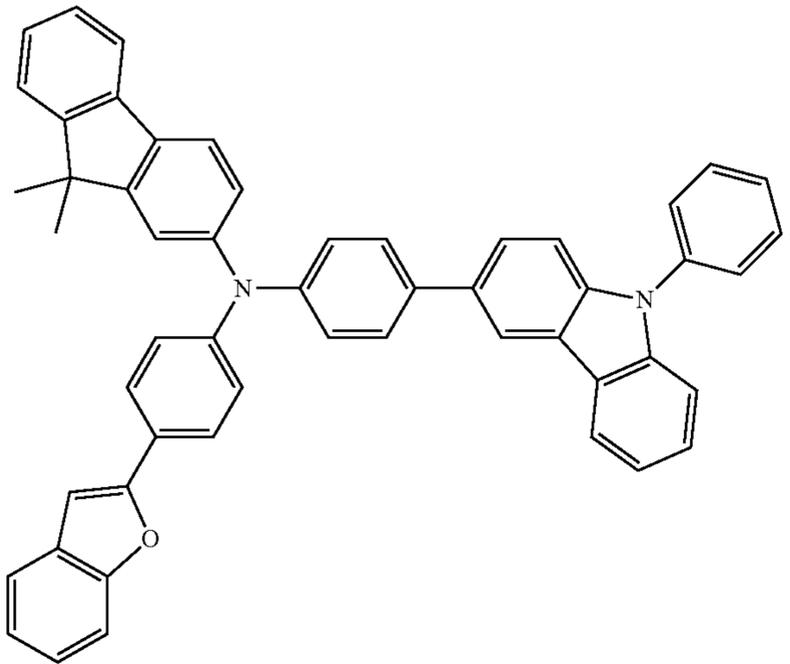
-continued



91

92

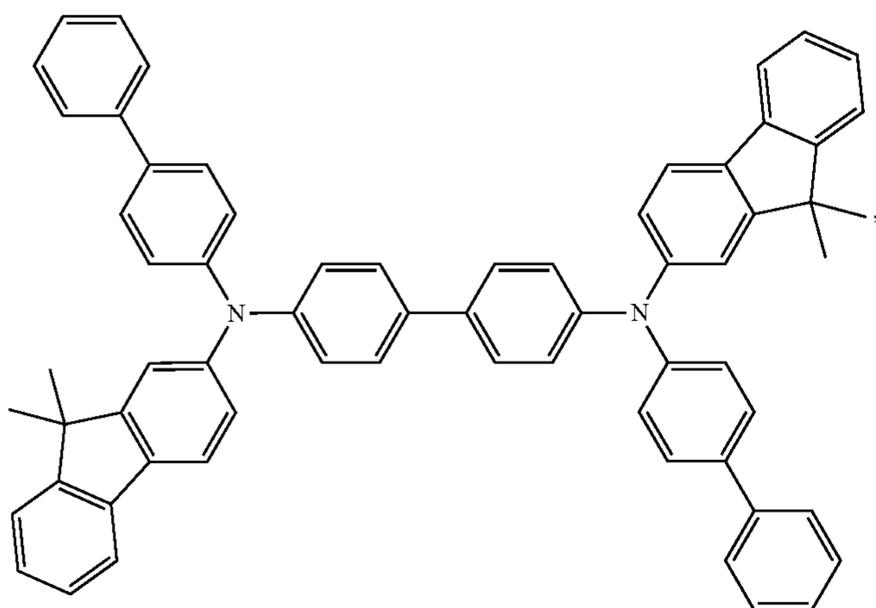
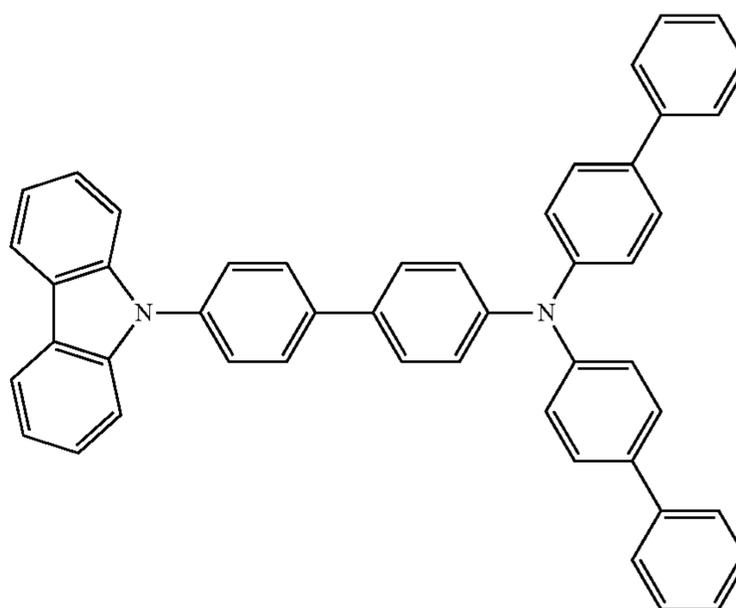
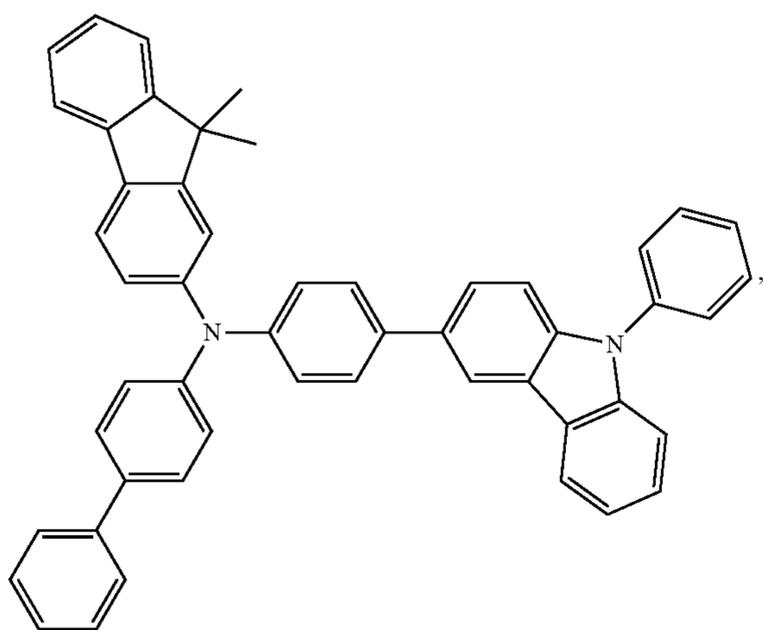
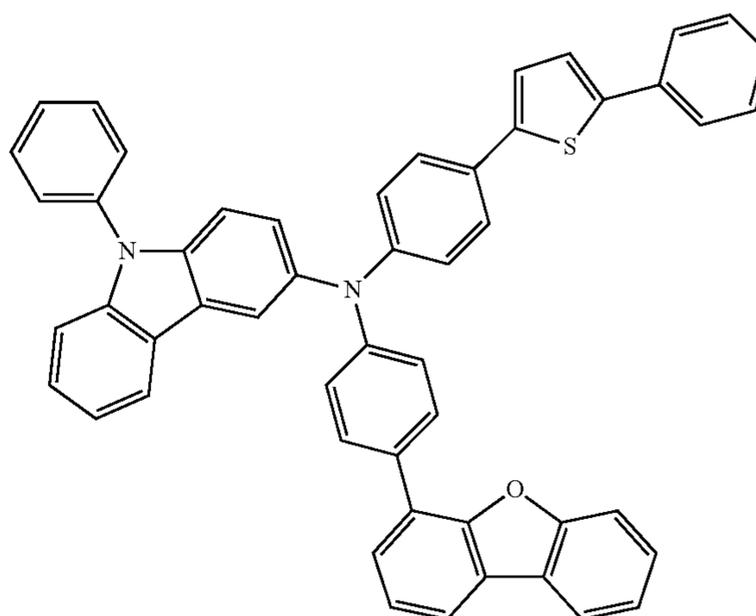
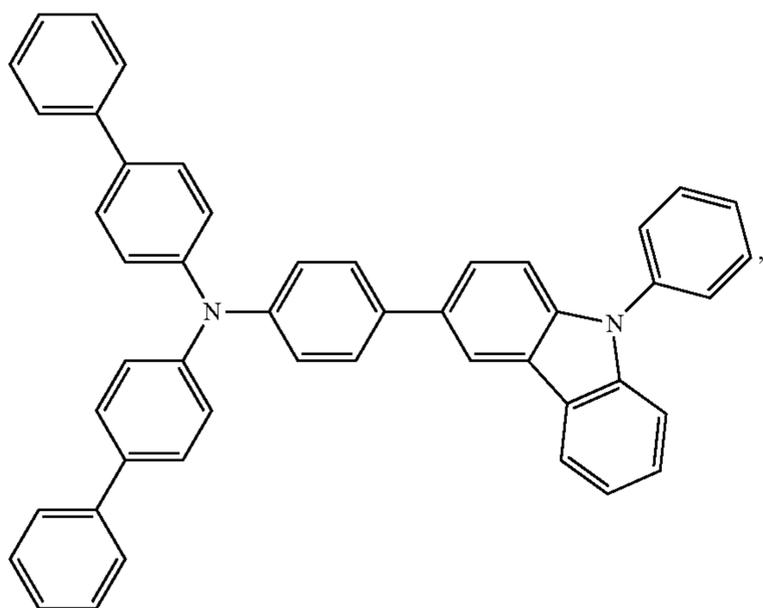
-continued



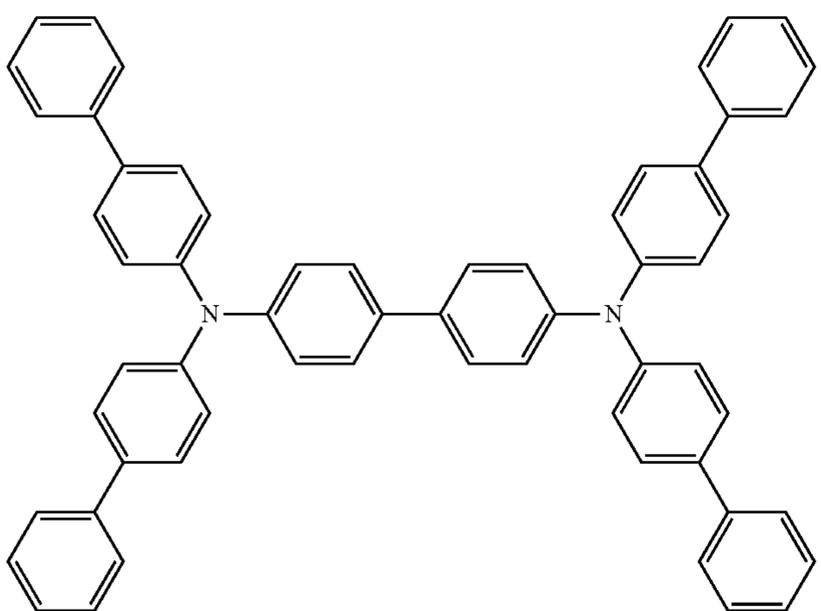
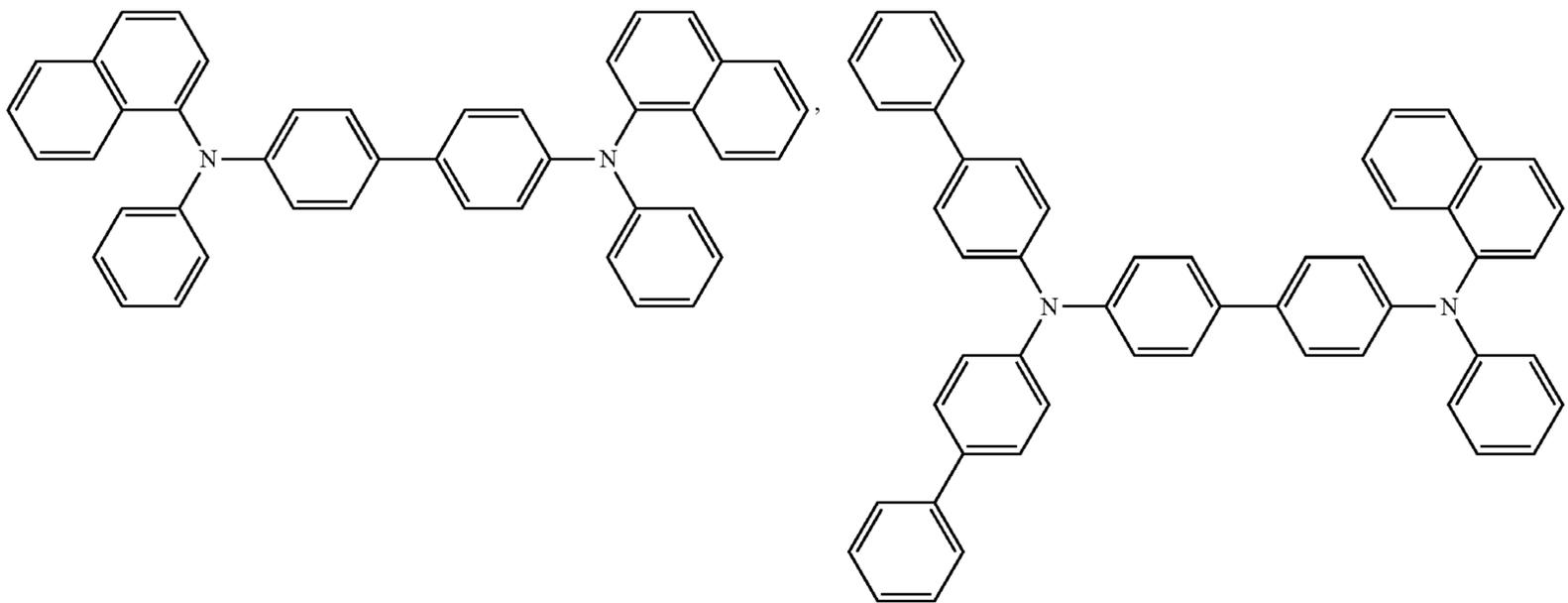
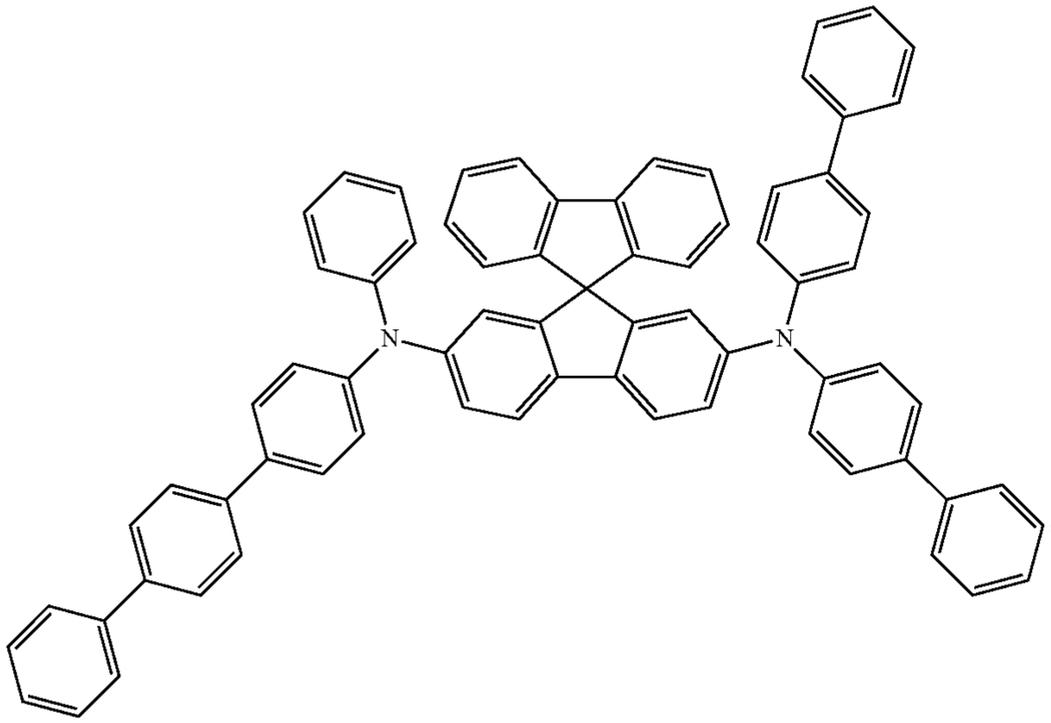
93

94

-continued



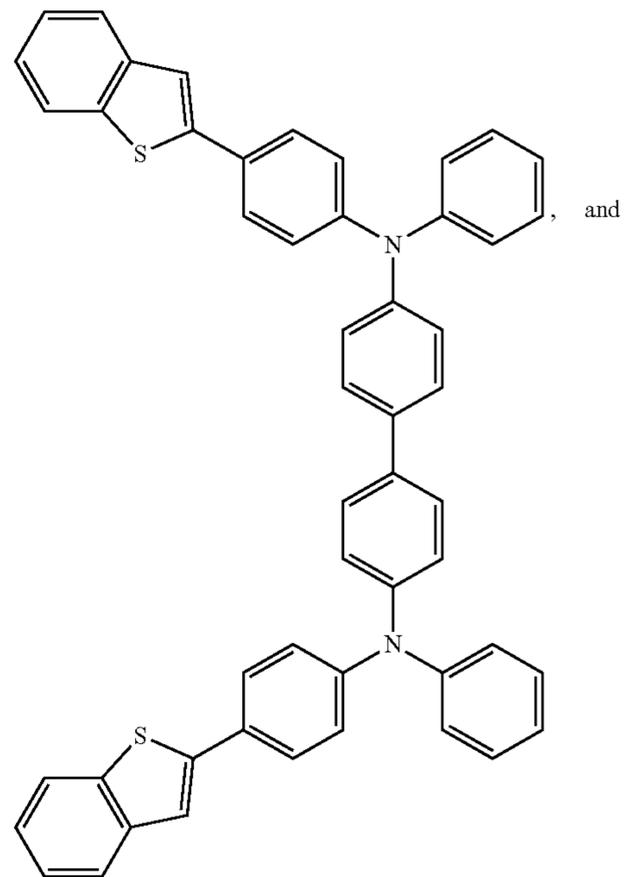
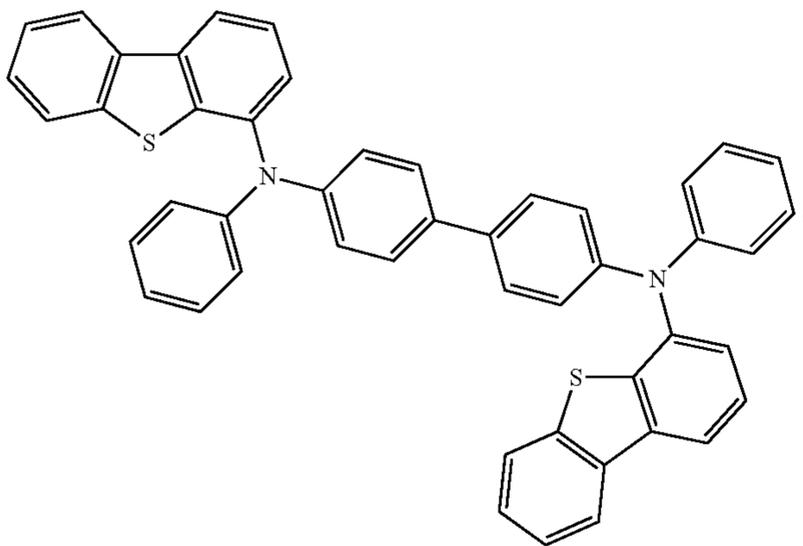
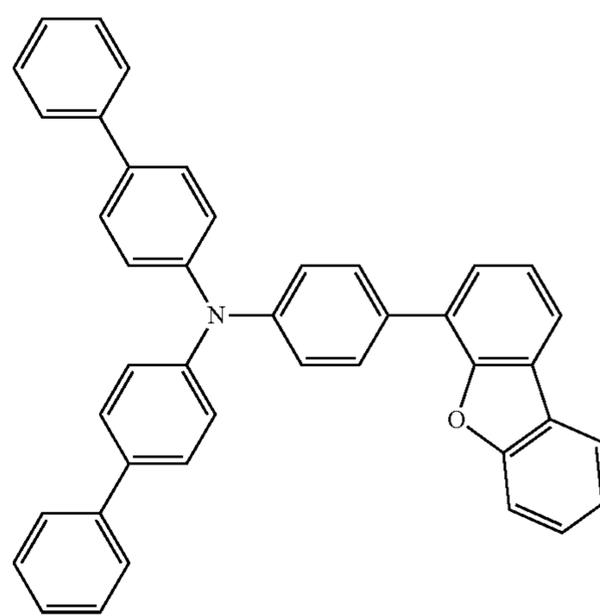
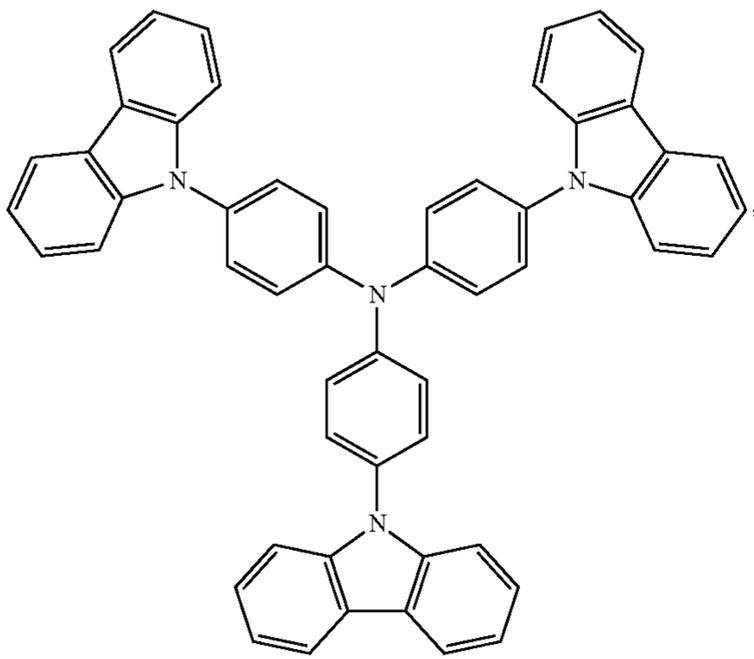
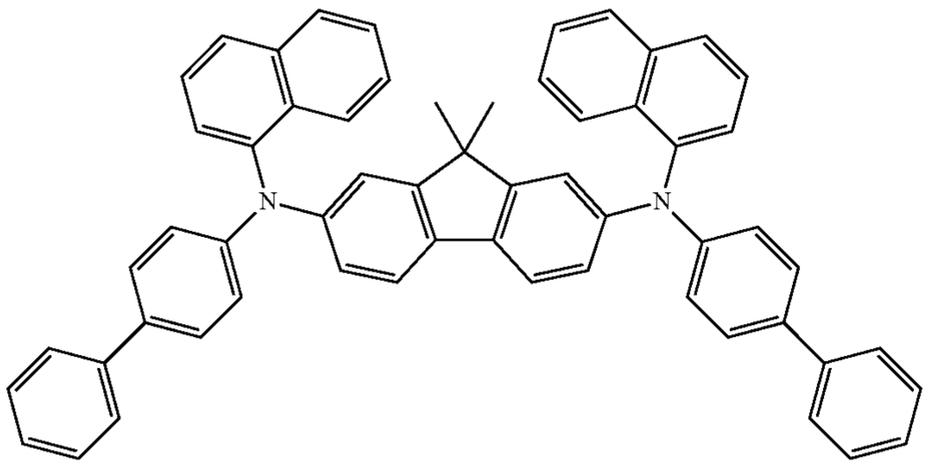
-continued



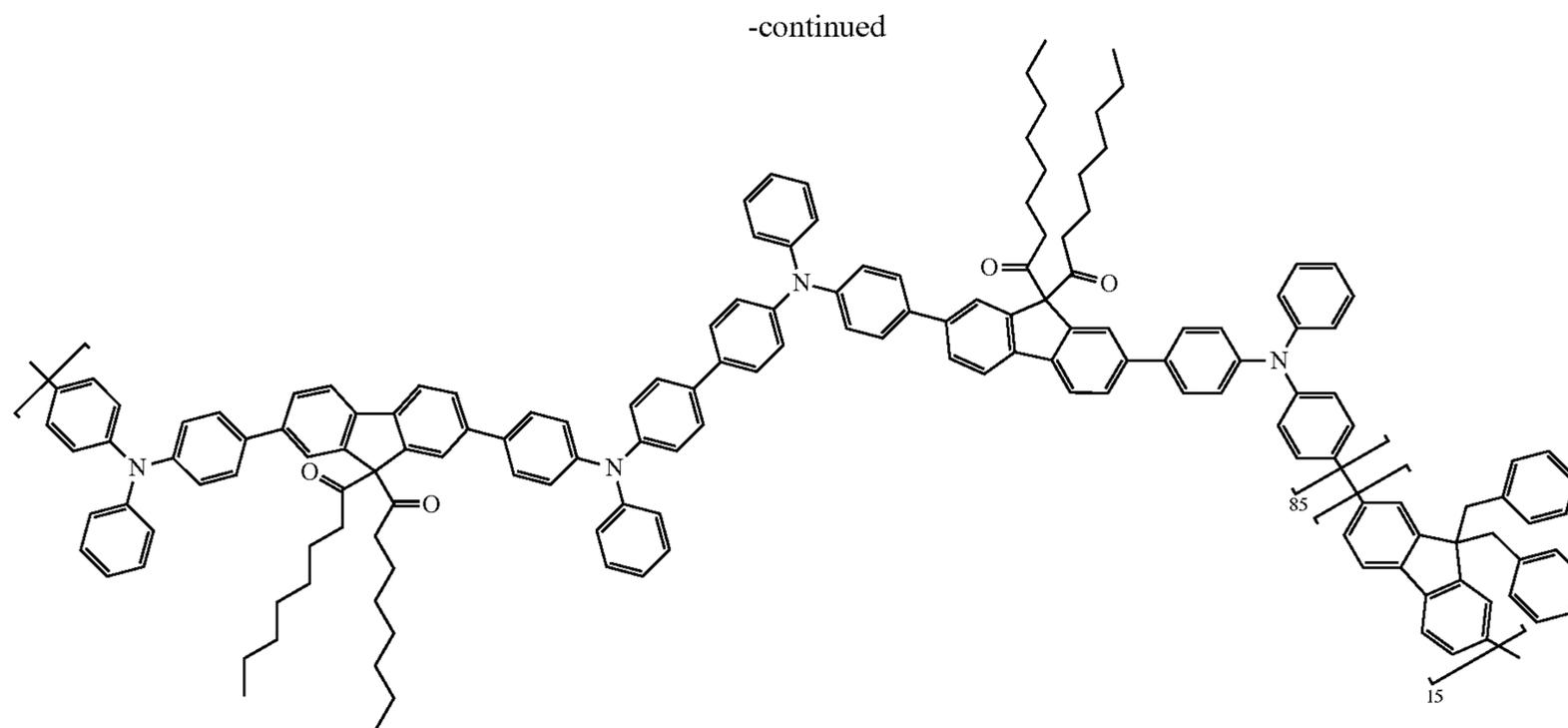
97

98

-continued



and



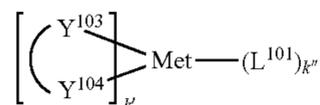
## EBL:

An electron blocking layer (EBL) may be used to reduce the number of electrons and/or excitons that leave the emissive layer. The presence of such a blocking layer in a device may result in substantially higher efficiencies, and or longer lifetime, as compared to a similar device lacking a blocking layer. Also, a blocking layer may be used to confine emission to a desired region of an OLED. In some embodiments, the EBL material has a higher LUMO (closer to the vacuum level) and/or higher triplet energy than the emitter closest to the EBL interface. In some embodiments, the EBL material has a higher LUMO (closer to the vacuum level) and or higher triplet energy than one or more of the hosts closest to the EBL interface. In one aspect, the compound used in EBL contains the same molecule or the same functional groups used as one of the hosts described below.

## Additional Hosts:

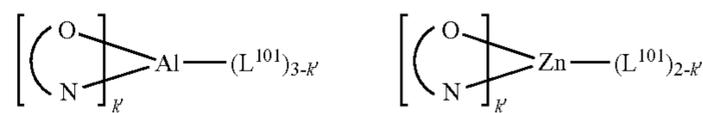
The light emitting layer of the organic EL device of the present invention preferably contains at least a metal complex as light emitting dopant material, and may contain one or more additional host materials using the metal complex as a dopant material. Examples of the host material are not particularly limited, and any metal complexes or organic compounds may be used as long as the triplet energy of the host is larger than that of the dopant. Any host material may be used with any dopant so long as the triplet criteria is satisfied.

Examples of metal complexes used as host are preferred to have the following general formula:



wherein Met is a metal; (Y<sup>103</sup>-Y<sup>104</sup>) is a bidentate ligand, Y<sup>103</sup> and Y<sup>104</sup> are independently selected from C, N, O, P, and S; L<sup>101</sup> is an another ligand; k' is an integer value from 1 to the maximum number of ligands that may be attached to the metal; and k'+k'' is the maximum number of ligands that may be attached to the metal.

In one aspect, the metal complexes are:



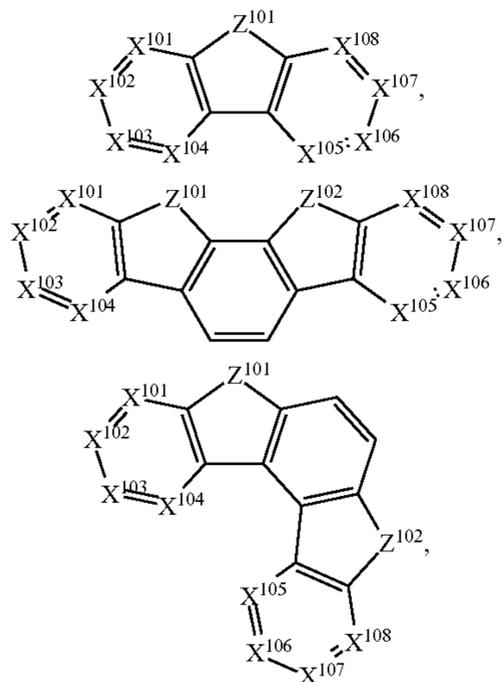
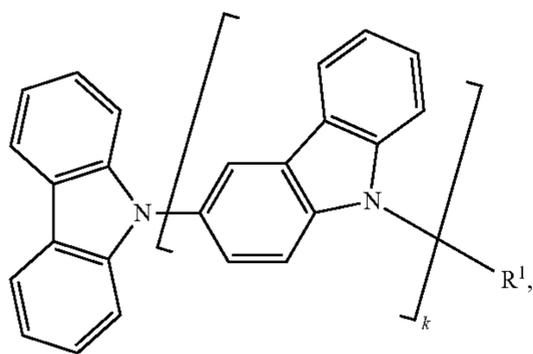
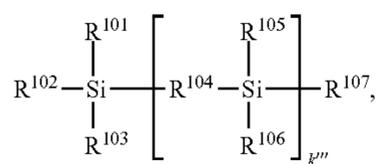
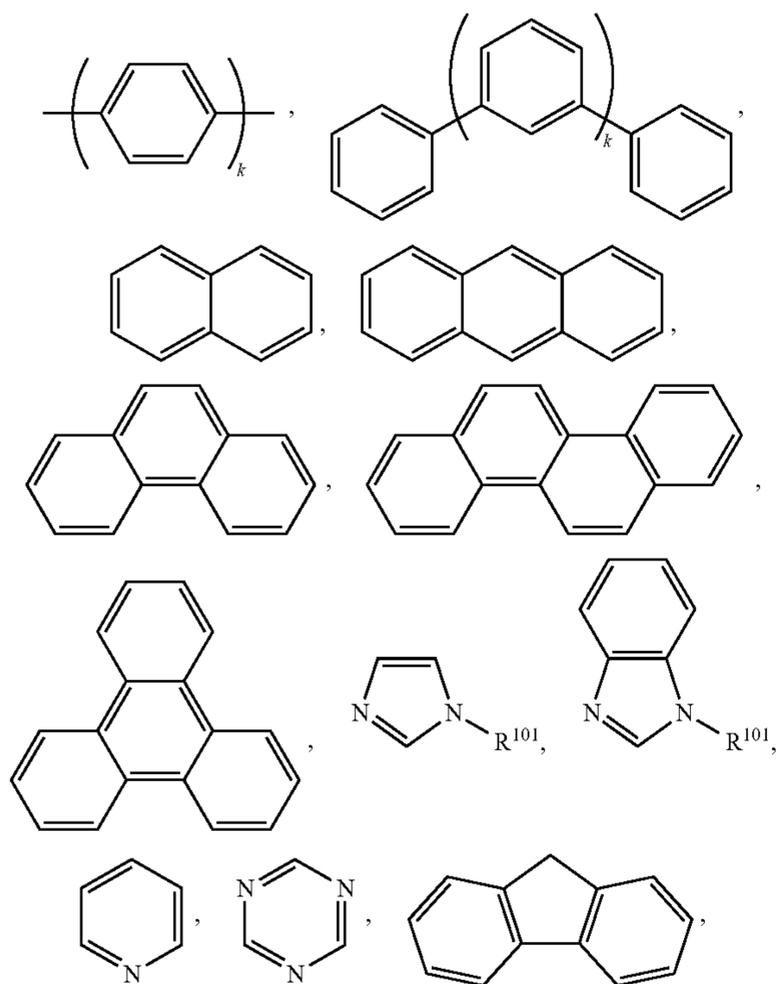
wherein (O—N) is a bidentate ligand, having metal coordinated to atoms O and N.

In another aspect, Met is selected from Ir and Pt. In a further aspect, (Y<sup>103</sup>-Y<sup>104</sup>) is a carbene ligand.

Examples of other organic compounds used as additional host are selected from the group consisting of aromatic hydrocarbon cyclic compounds such as benzene, biphenyl, triphenyl, triphenylene, naphthalene, anthracene, phenalene, phenanthrene, fluorene, pyrene, chrysene, perylene, azulene; group consisting aromatic heterocyclic compounds such as dibenzothiophene, dibenzofuran, dibenzoselenophene, furan, thiophene, benzofuran, benzothiophene, benzoselenophene, carbazole, indolocarbazole, pyridylindole, pyrrolodipyridine, pyrazole, imidazole, triazole, oxazole, thiazole, oxadiazole, oxatriazole, dioxazole, thiadiazole, pyridine, pyridazine, pyrimidine, pyrazine, triazine, oxazine, oxathiazine, oxadiazine, indole, benzimidazole, indazole, indoxazine, benzoxazole, benzisoxazole, benzothiazole, quinoline, isoquinoline, cinnoline, quinazoline, quinoxaline, naphthyridine, phthalazine, pteridine, xanthene, acridine, phenazine, phenothiazine, phenoxazine, benzofuropyridine, furodipyridine, benzothienopyridine, thienodipyridine, benzoselenophenopyridine, and selenophenodipyridine; and group consisting 2 to 10 cyclic structural units which are groups of the same type or different types selected from the aromatic hydrocarbon cyclic group and the aromatic heterocyclic group and are bonded to each other directly or via at least one of oxygen atom, nitrogen atom, sulfur atom, silicon atom, phosphorus atom, boron atom, chain structural unit and the aliphatic cyclic group. Wherein each group is further substituted by a substituent selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, arvloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof.

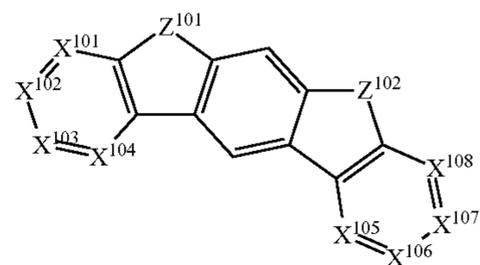
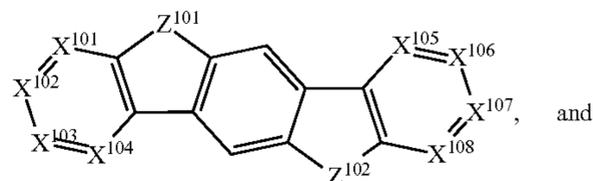
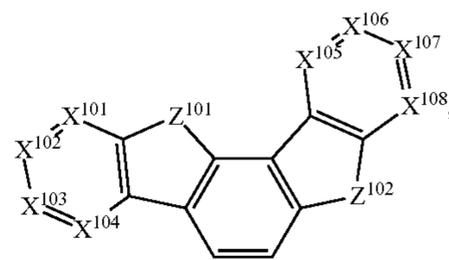
In one aspect, host compound contains at least one of the following groups in the molecule:

101



102

-continued



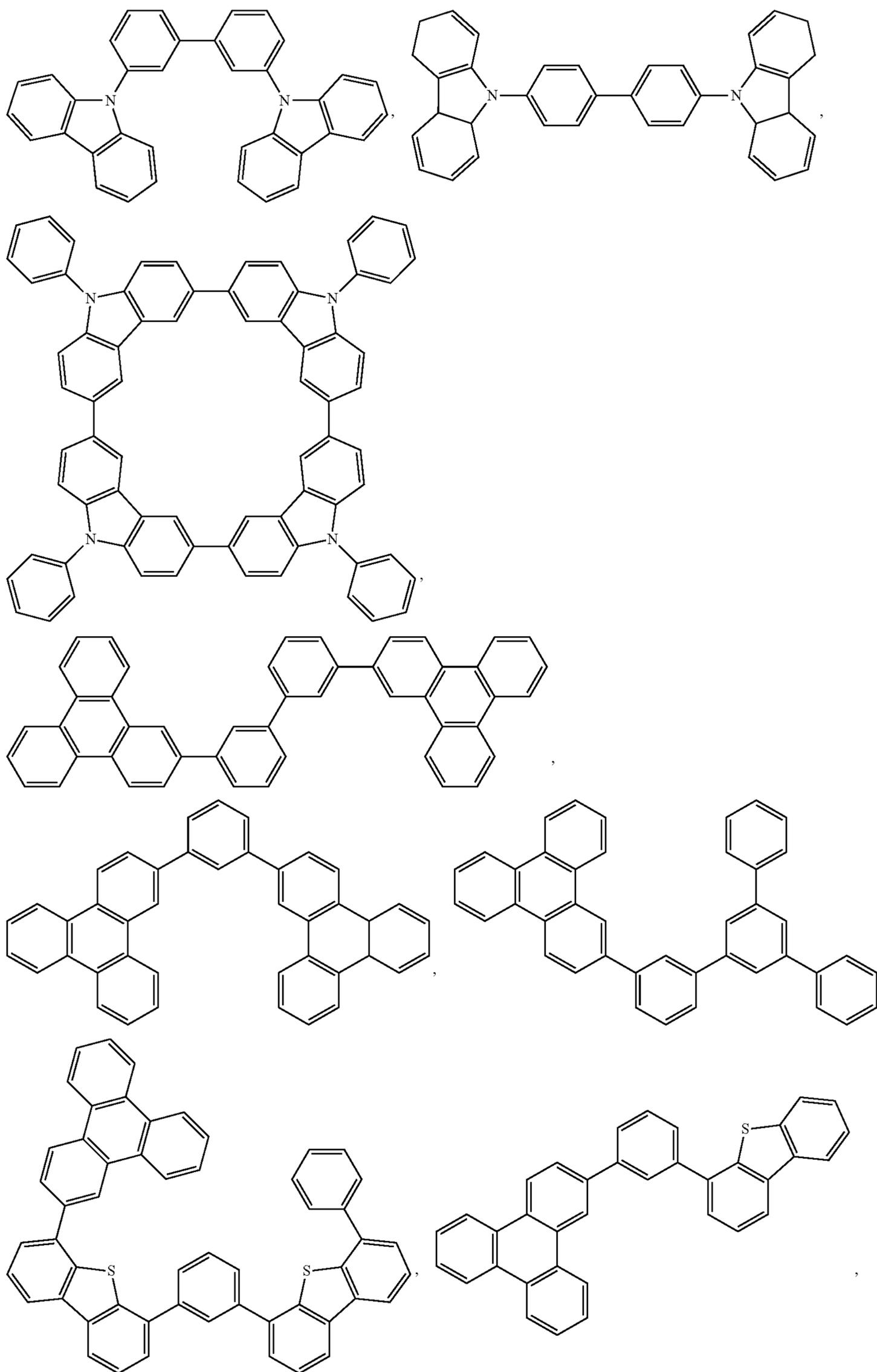
wherein  $R^{101}$  to  $R^{107}$  is independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof, when it is aryl or heteroaryl, it has the similar definition as Ar's mentioned above.  $k$  is an integer from 0 to 20 or 1 to 20.  $k'''$  is an integer from 0 to 20.  $X^{101}$  to  $X^{108}$  is selected from C (including CH) or N.

$Z^{101}$  and  $Z^{102}$  is selected from  $NR^{101}$ , O, or S.

Non-limiting examples of the additional host materials that may be used in an OLED in combination with the host compound disclosed herein are exemplified below together with references that disclose those materials: EP2034538, EP2034538A, EP2757608, JP2007254297, KR20100079458, KR20120088644, KR20120129733, KR20130115564, TW201329200, US20030175553, US20050238919, US20060280965, US20090017330, US20090030202, US20090167162, US20090302743, US20090309488, US20100012931, US20100084966, US20100187984, US2010187984, US2012075273, US2012126221, US2013009543, US2013105787, US2013175519, US2014001446, US20140183503, US20140225088, US2014034914, U.S. Pat. No. 7,154,114, WO2001039234, WO2004093207, WO2005014551, WO2005089025, WO2006072002, WO2006114966, WO2007063754, WO2008056746, WO2009003898, WO2009021126, WO2009063833, WO2009066778, WO2009066779, WO2009086028, WO2010056066, WO2010107244, WO2011081423, WO2011081431, WO2011086863, WO2012128298, WO2012133644, WO2012133649, WO2013024872, WO2013035275, WO2013081315, WO2013191404, WO2014142472,

103

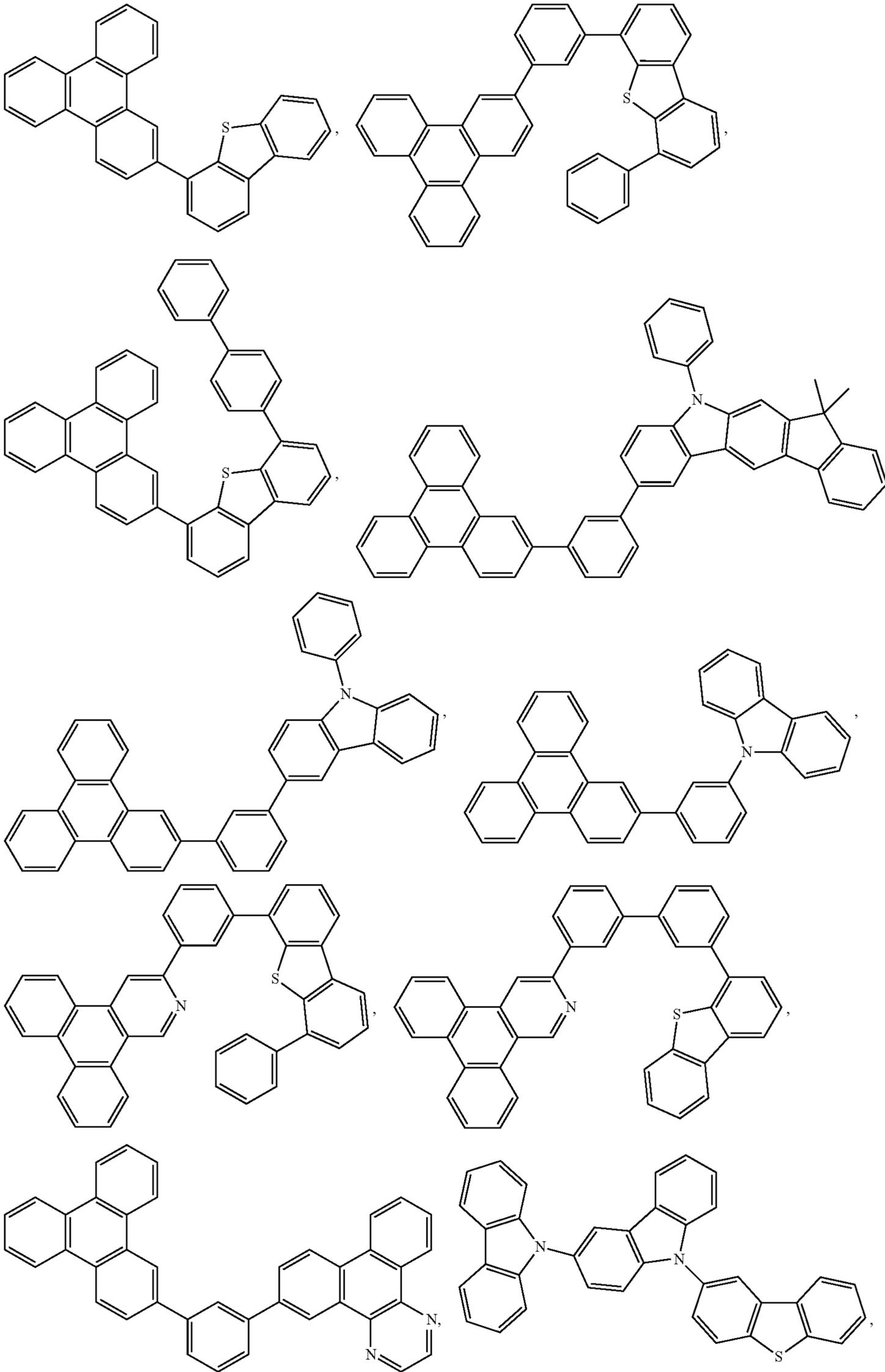
104



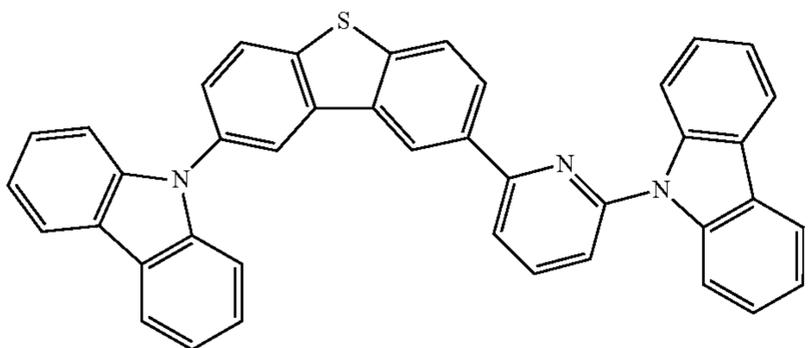
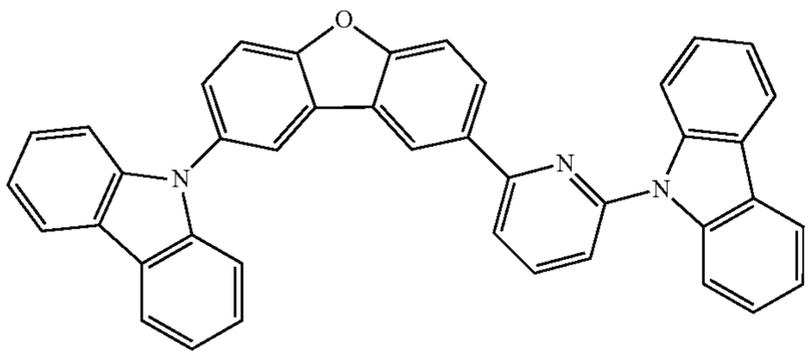
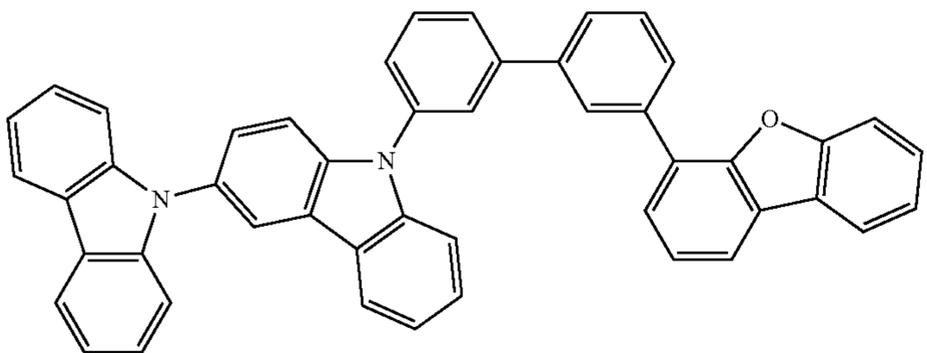
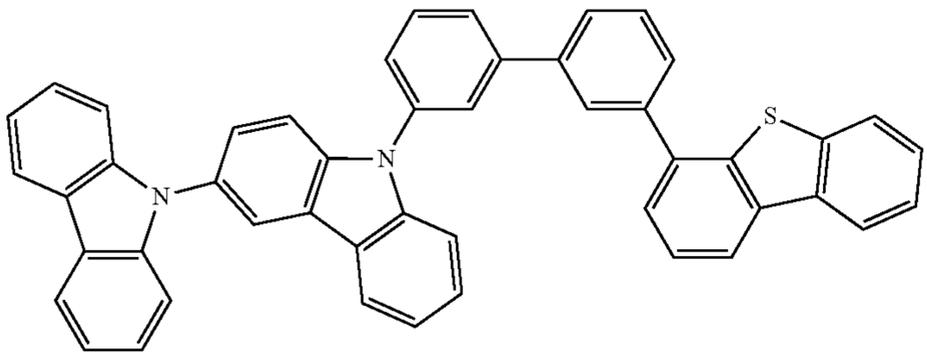
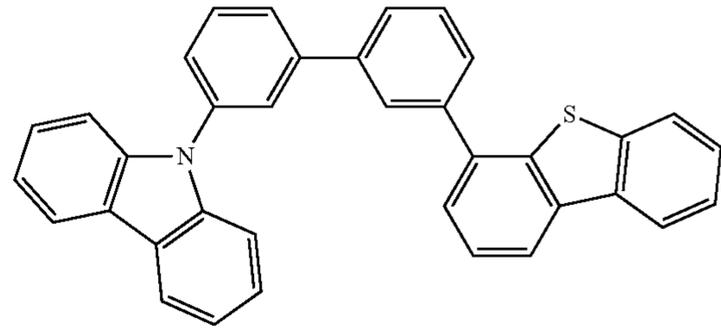
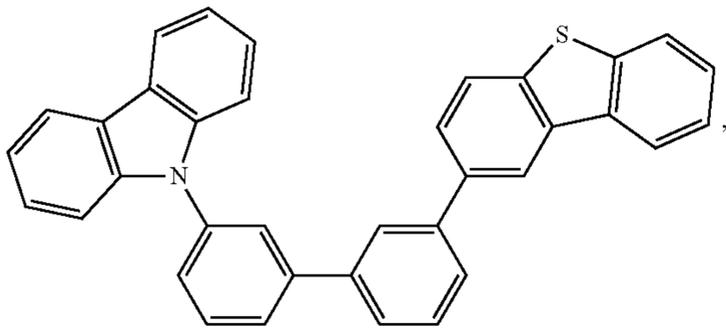
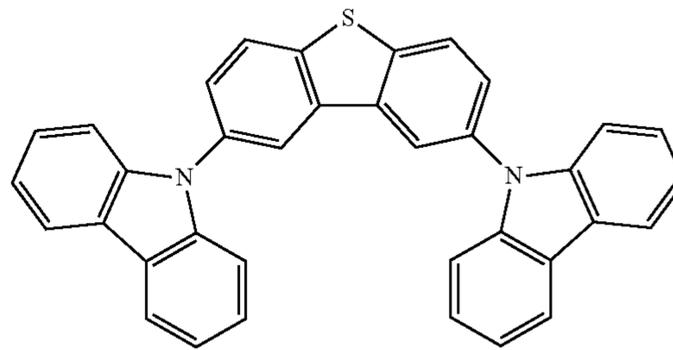
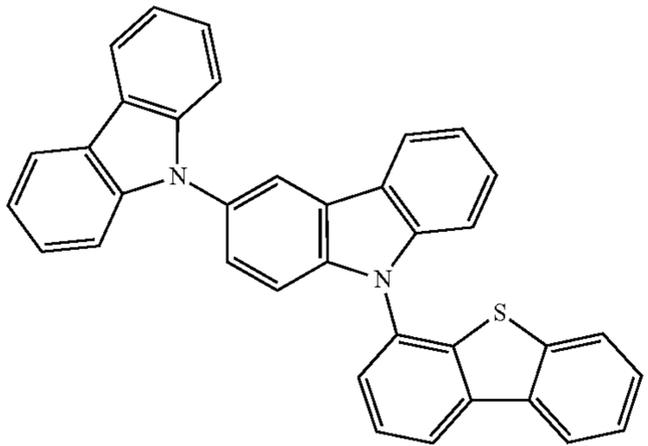
105

106

-continued

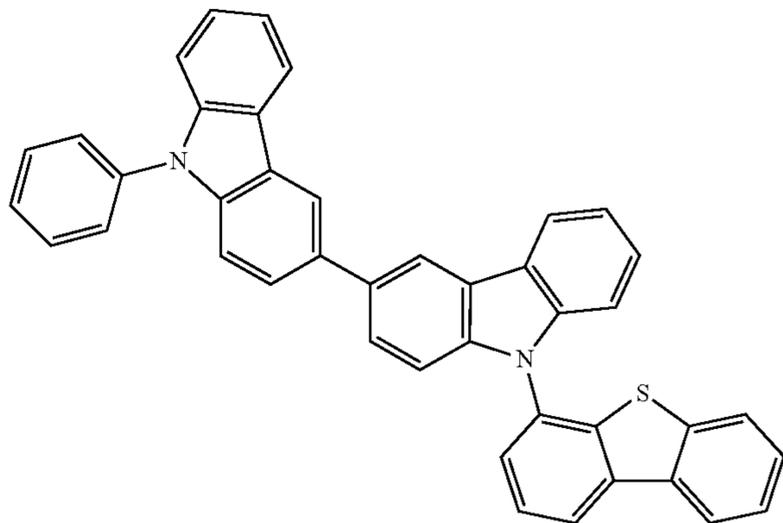
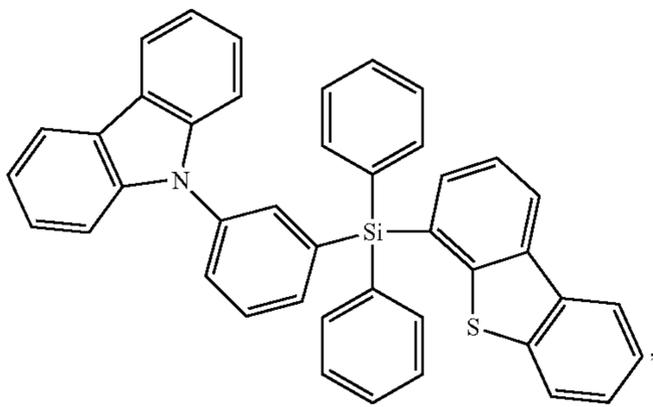
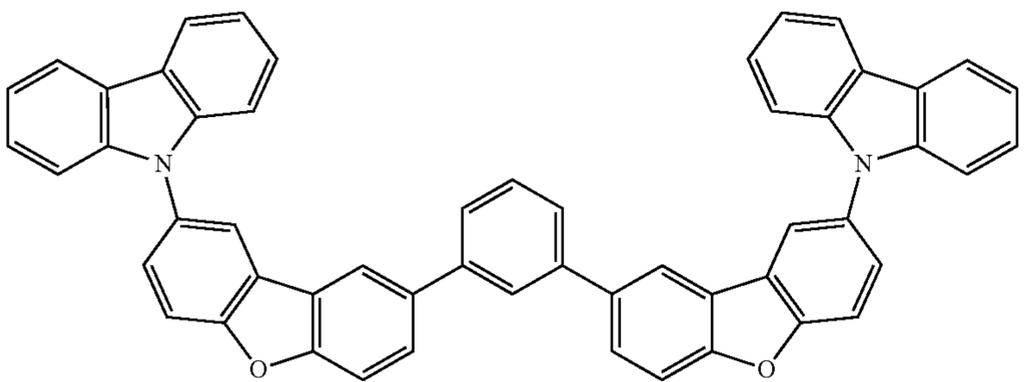
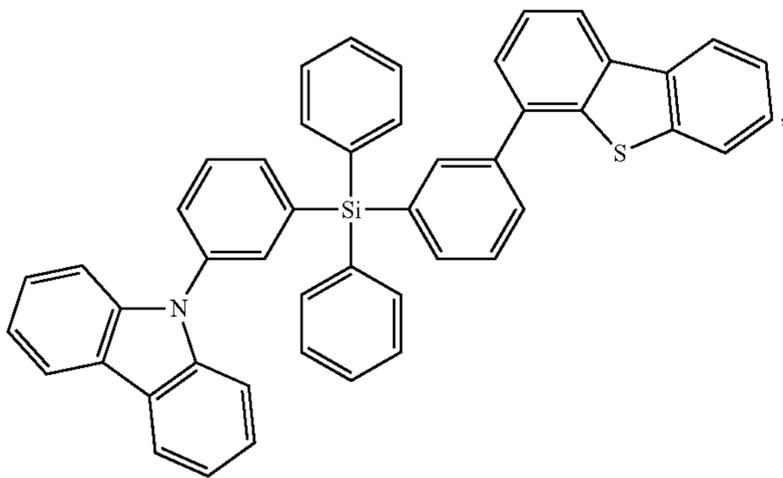
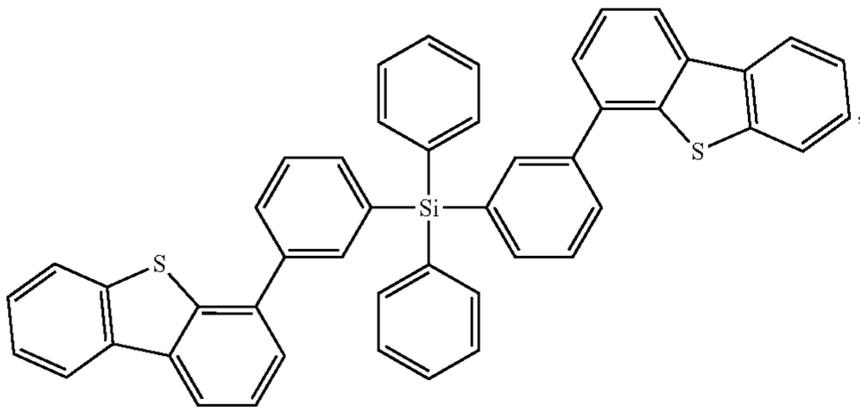
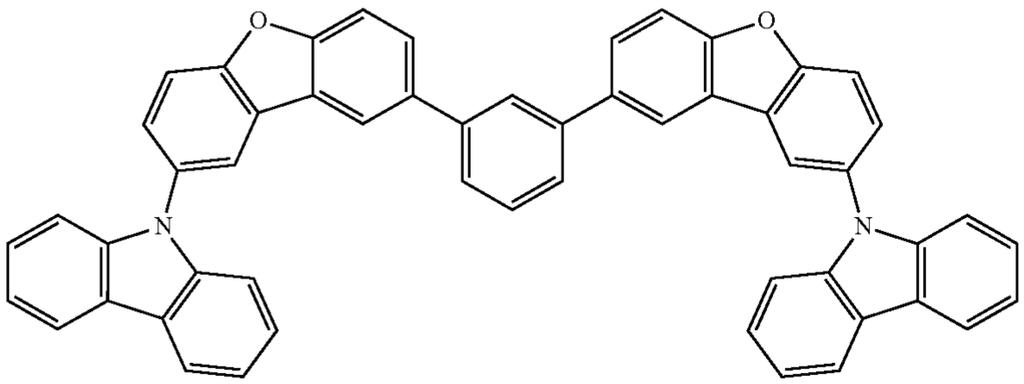


-continued

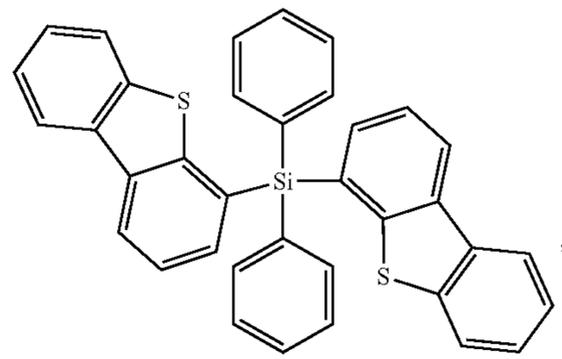


109

-continued



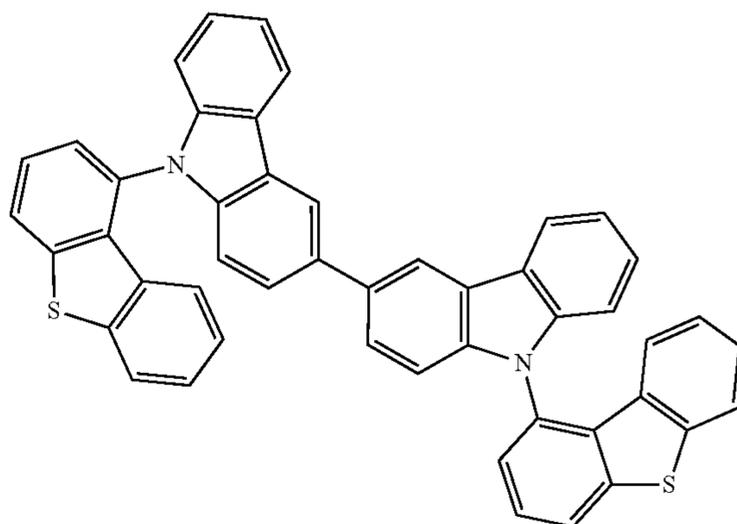
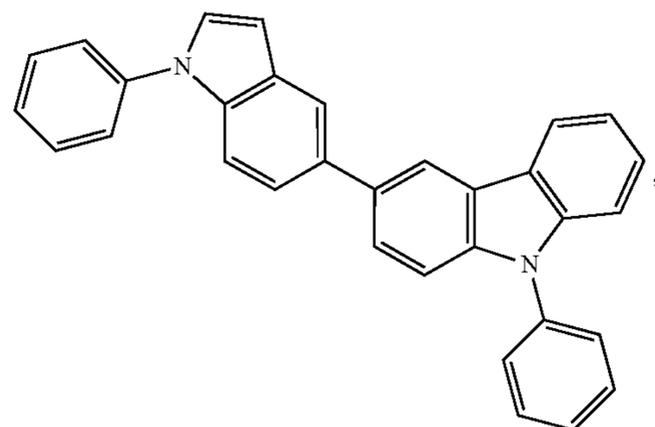
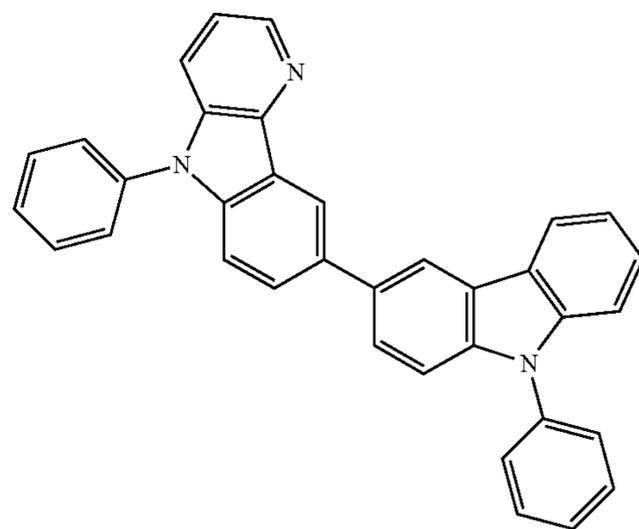
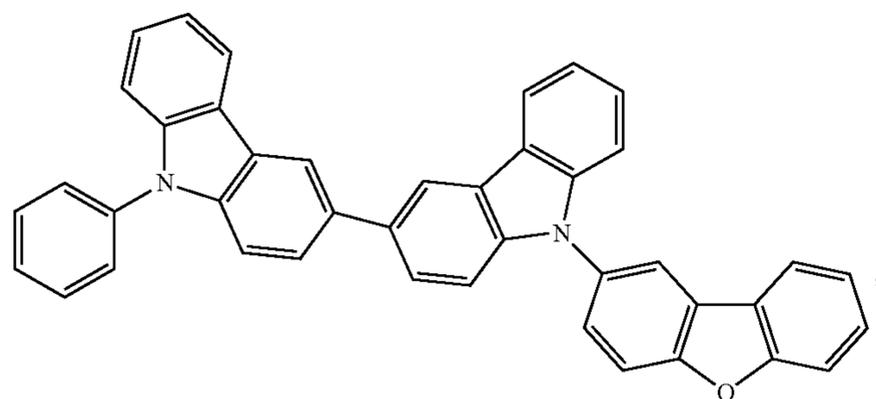
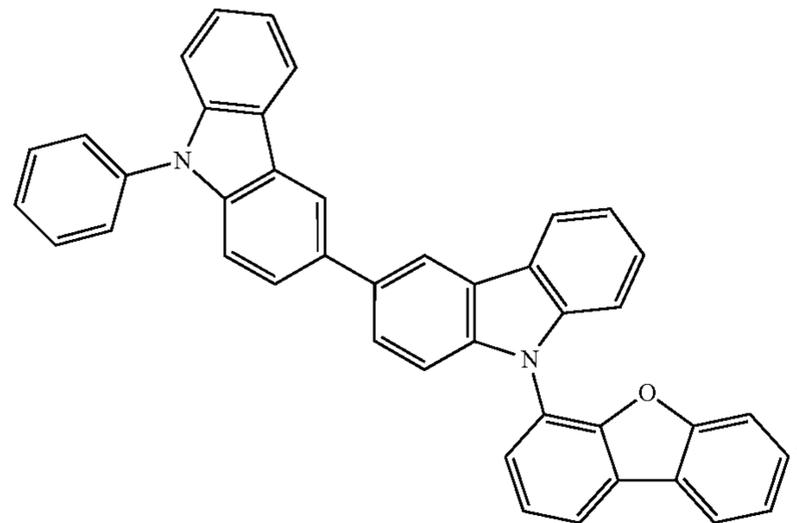
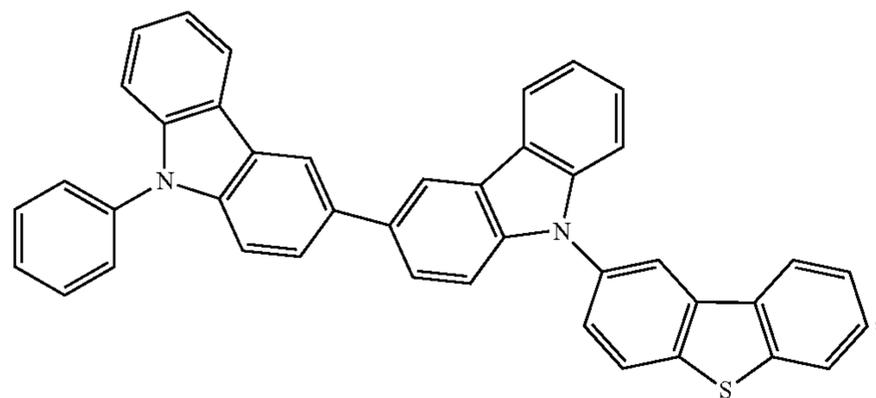
110



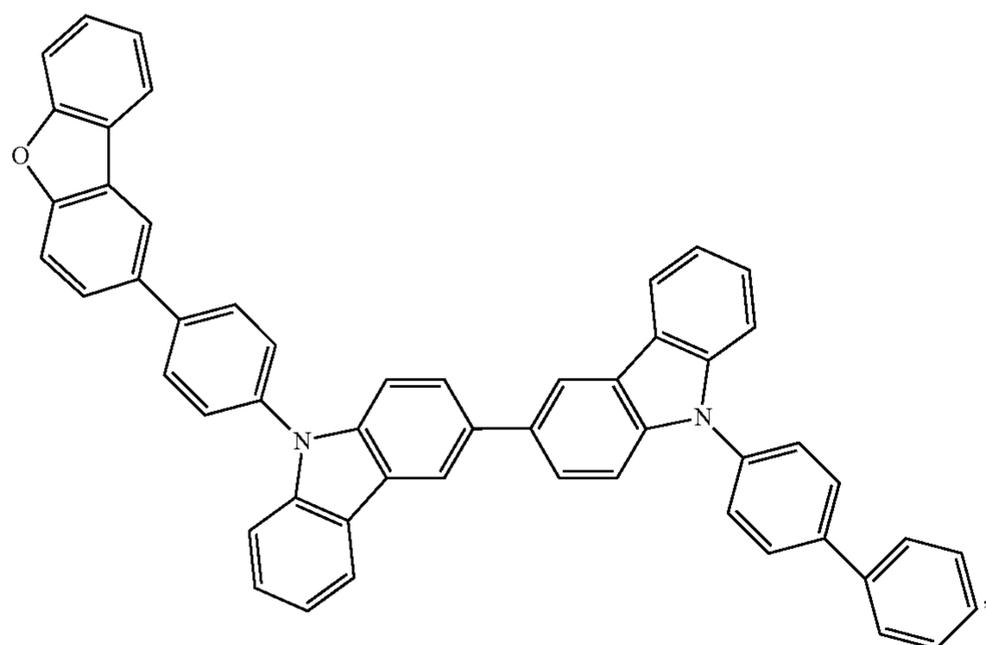
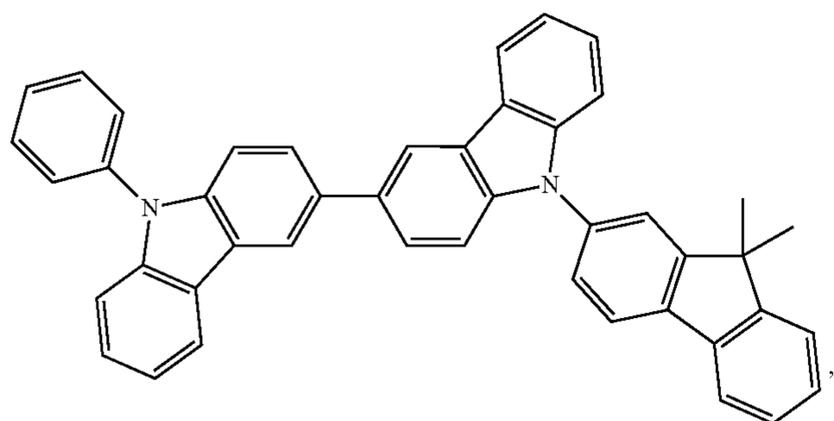
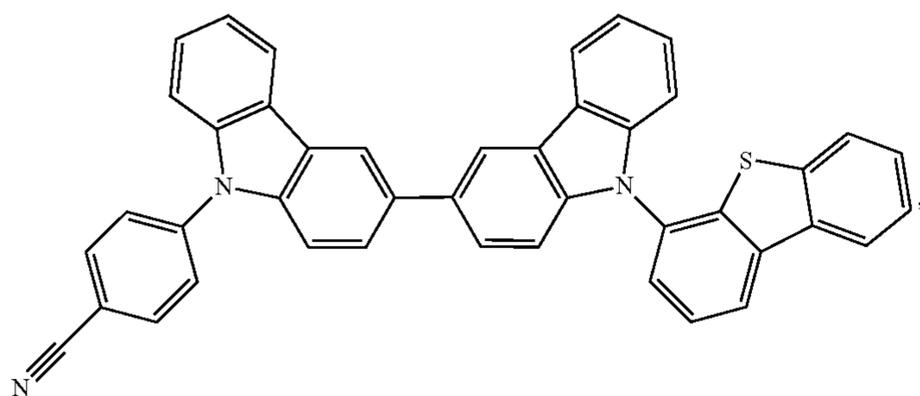
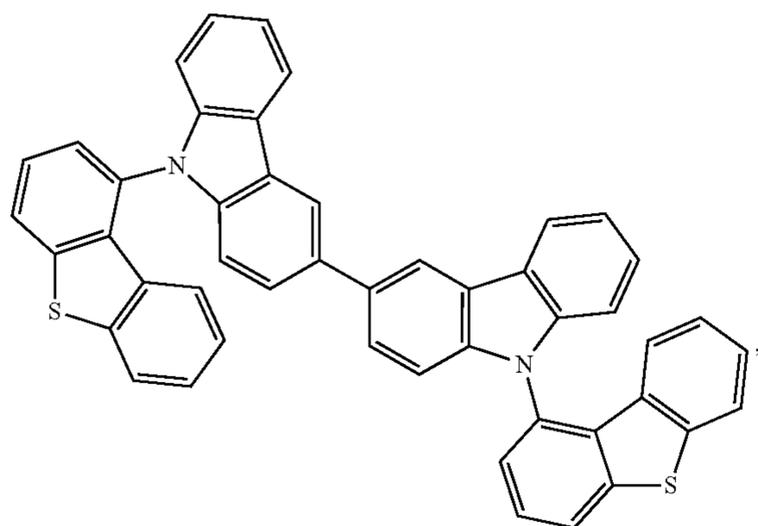
111

112

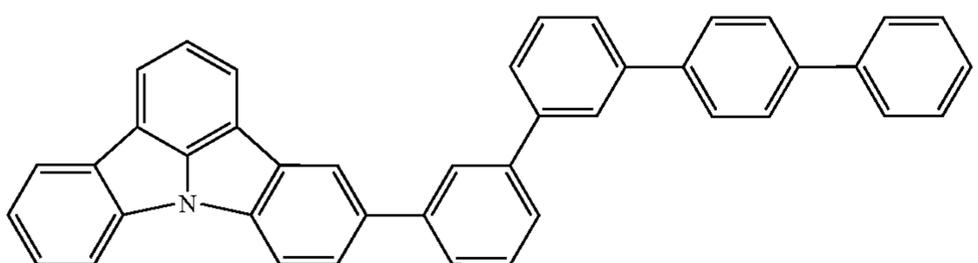
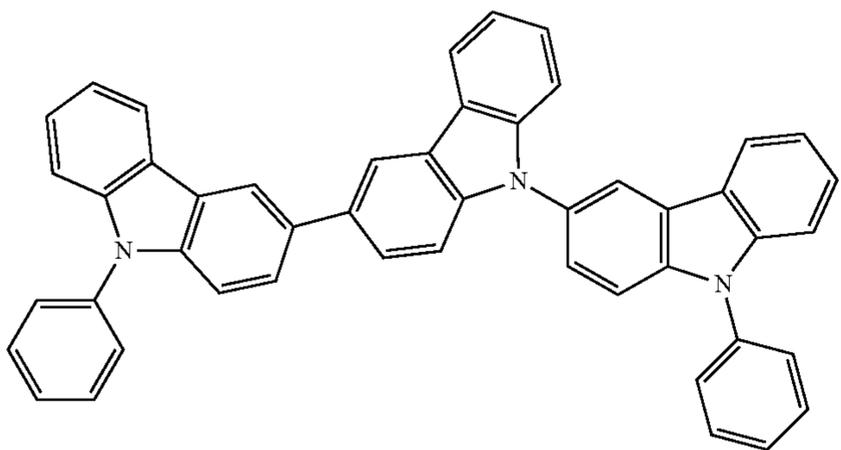
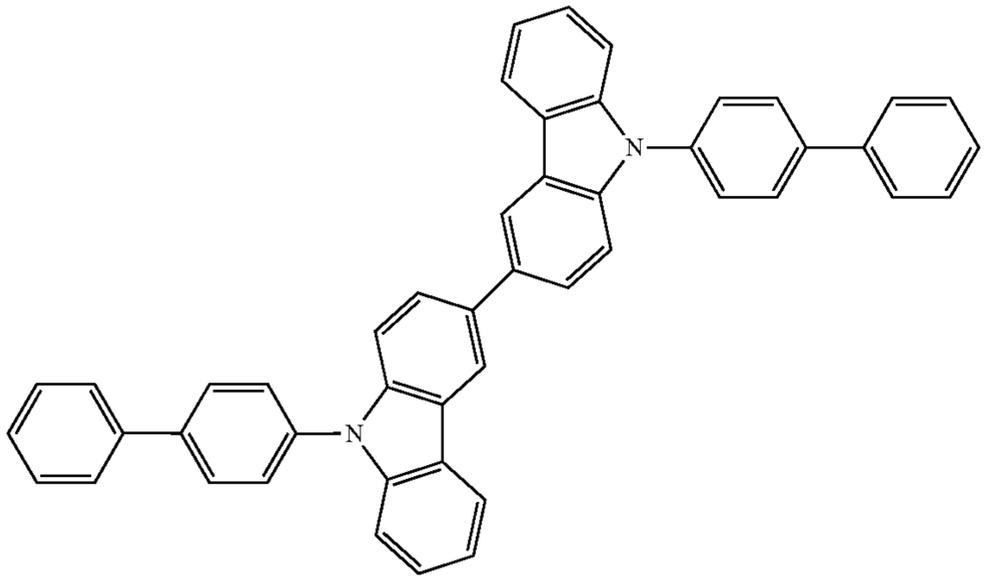
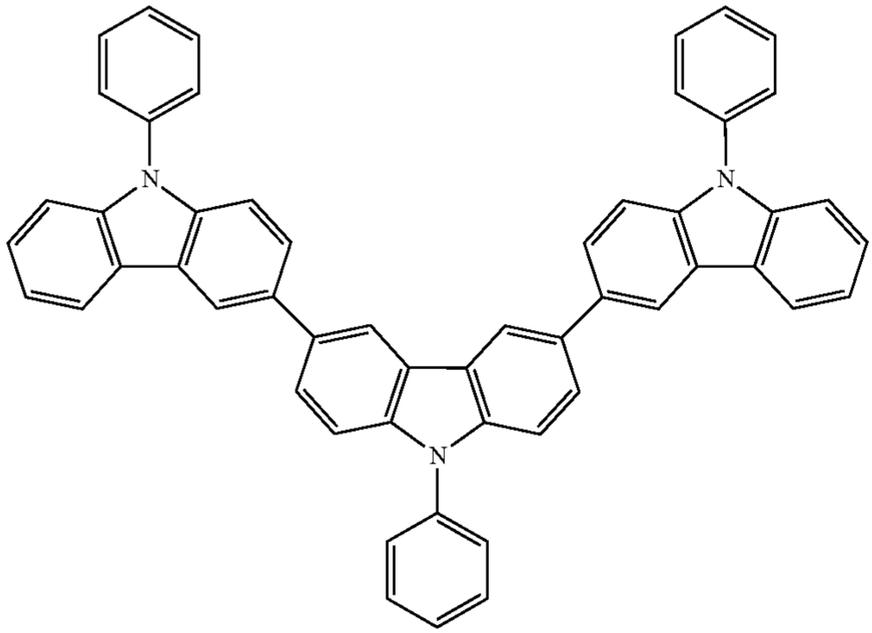
-continued



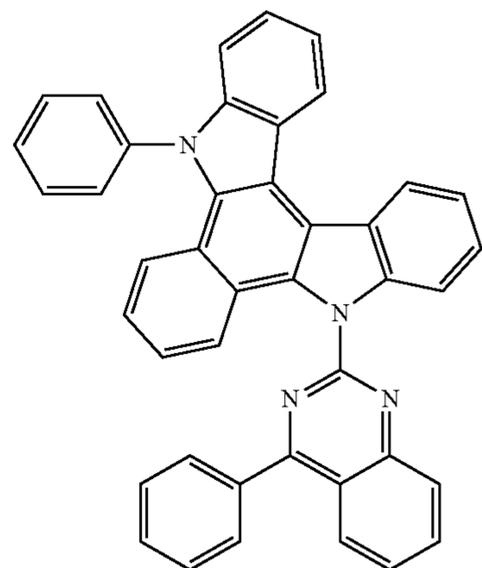
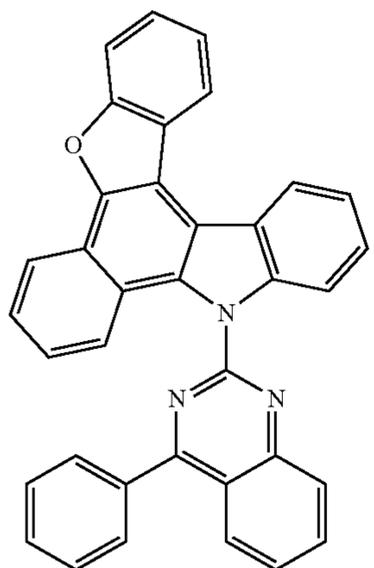
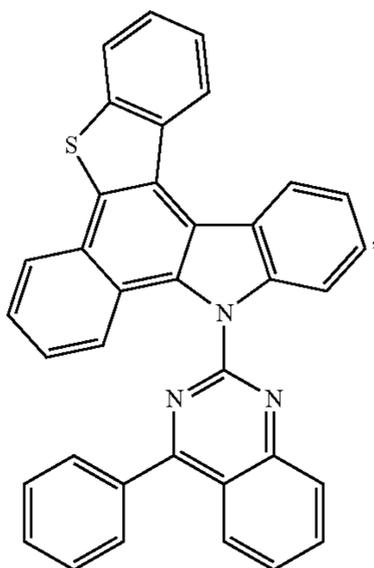
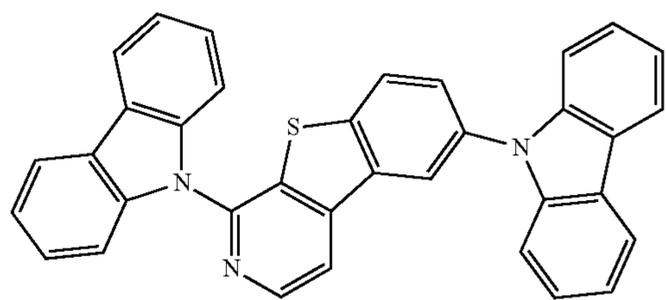
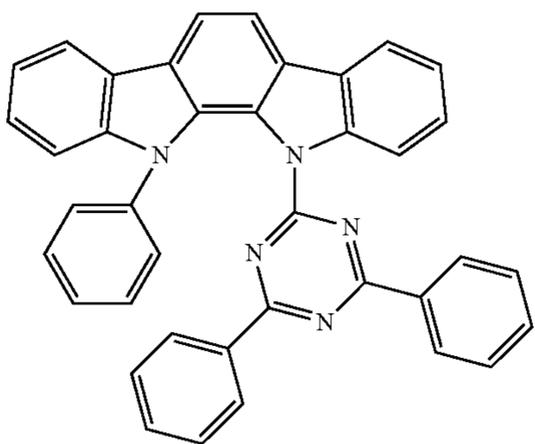
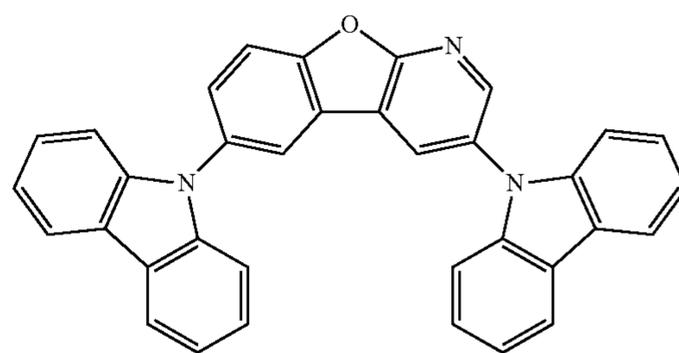
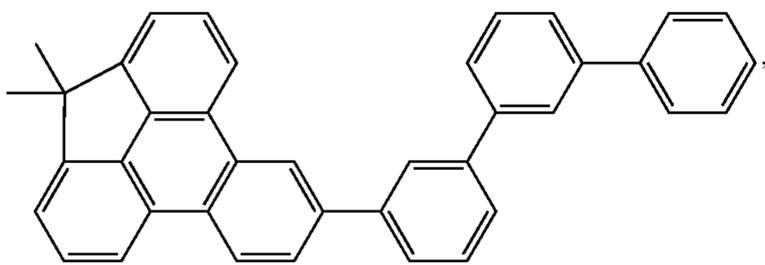
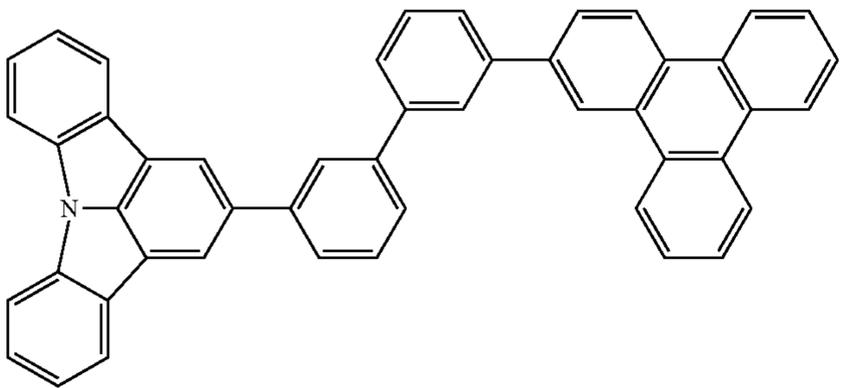
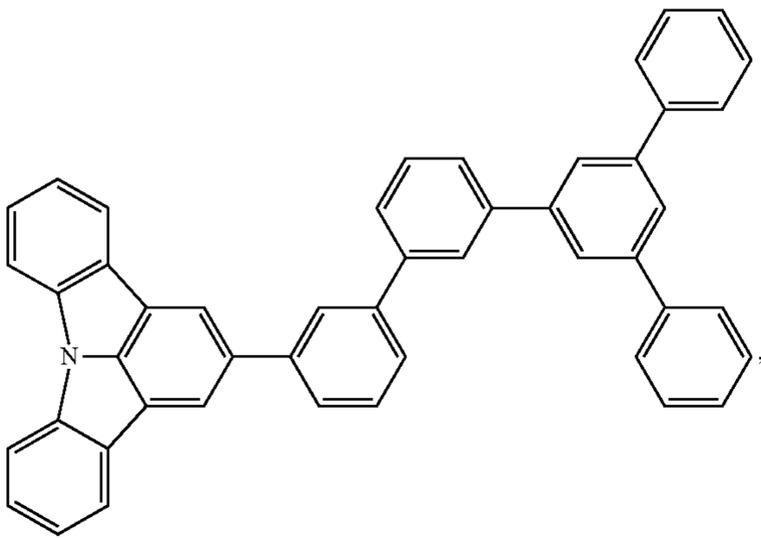
-continued



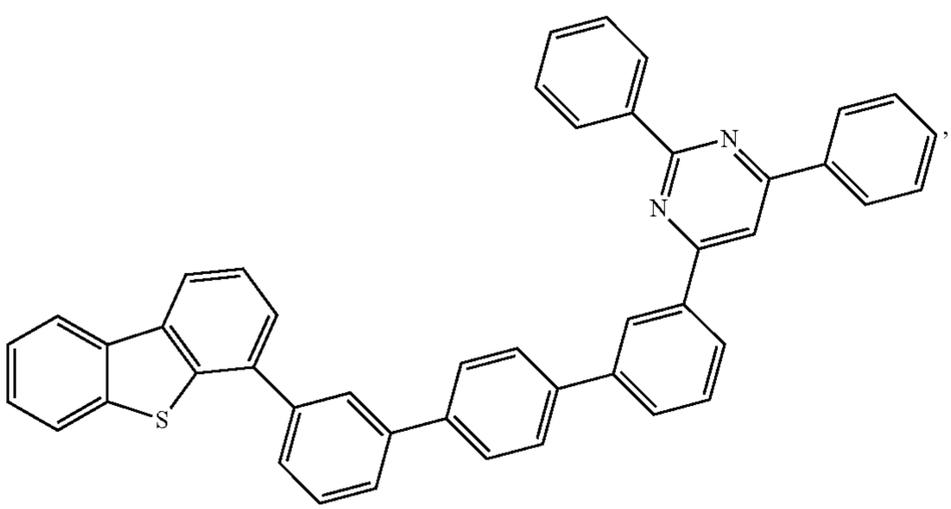
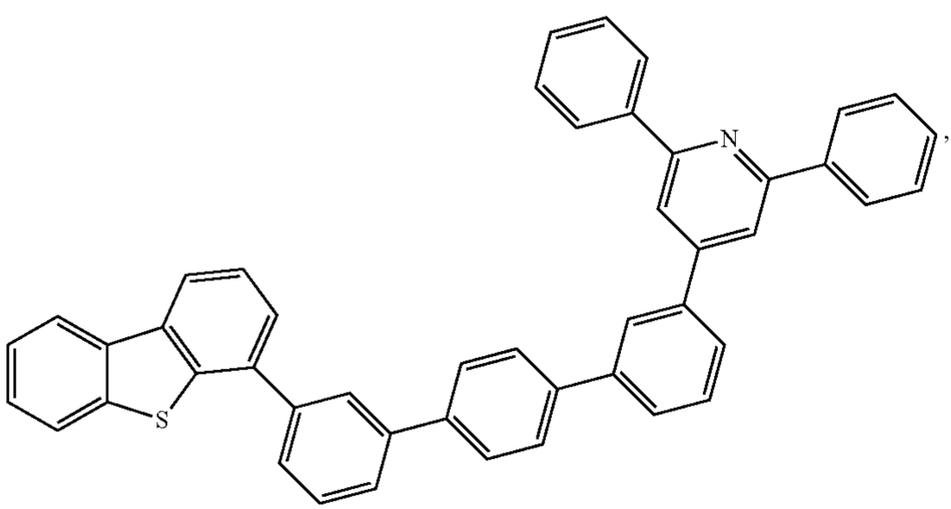
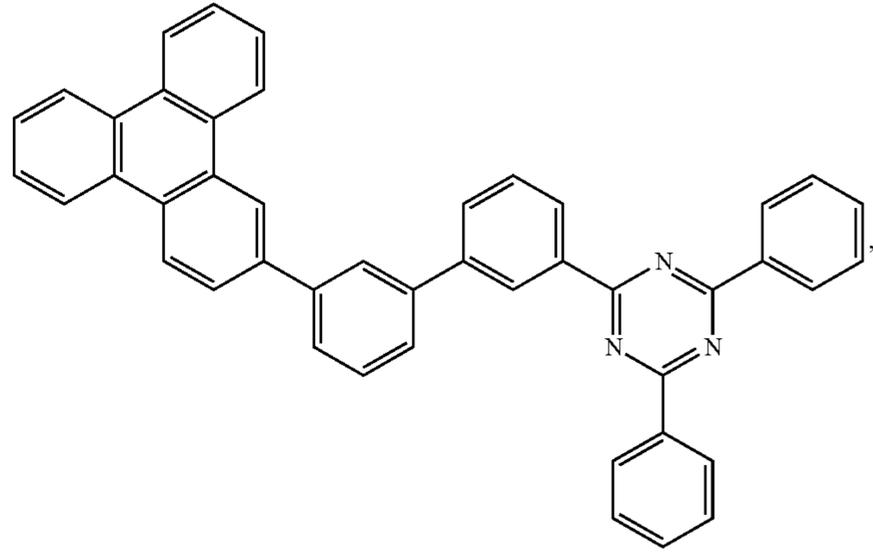
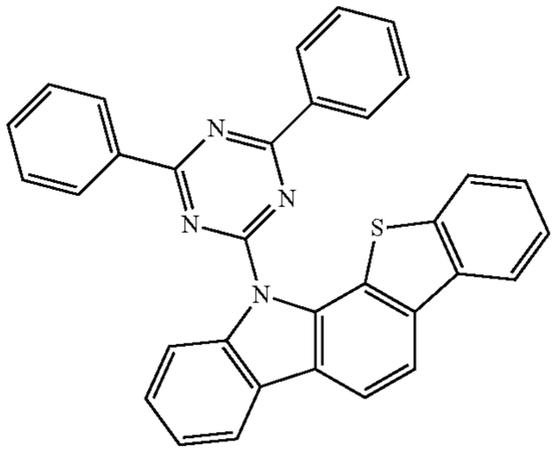
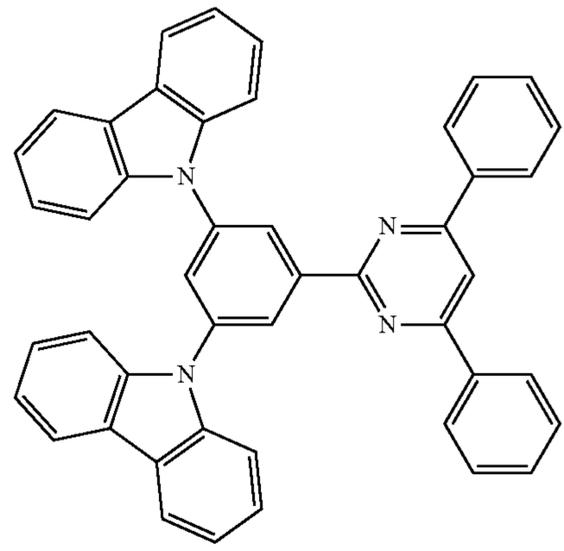
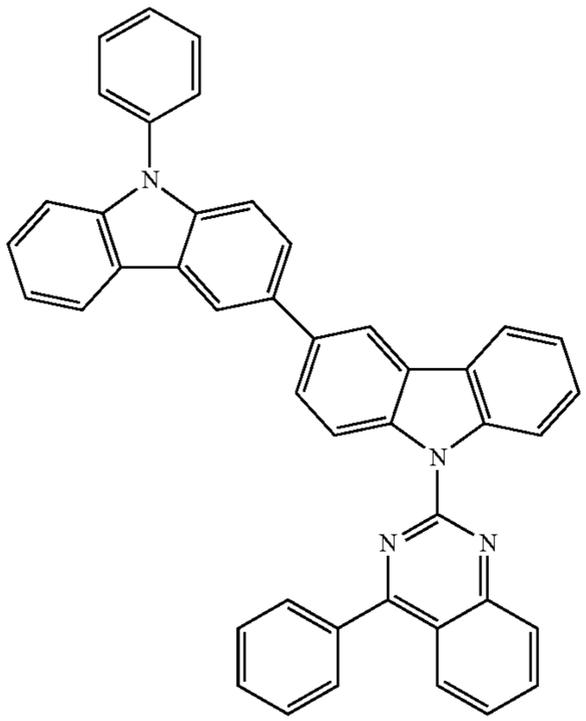
-continued



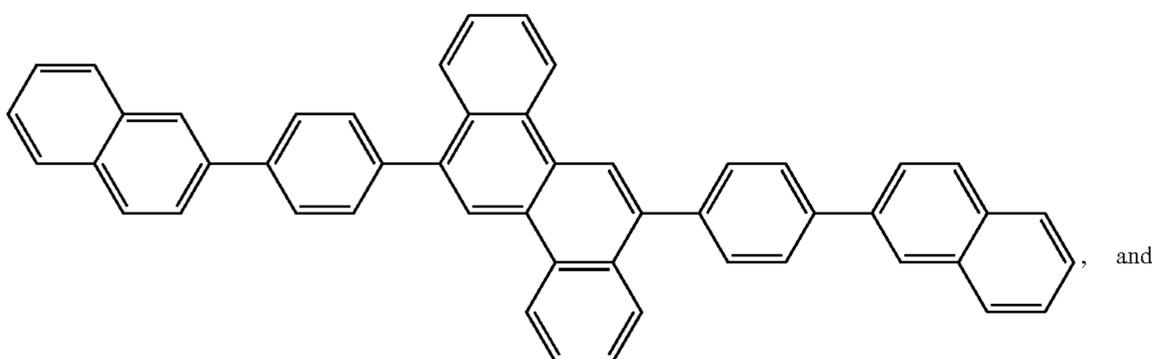
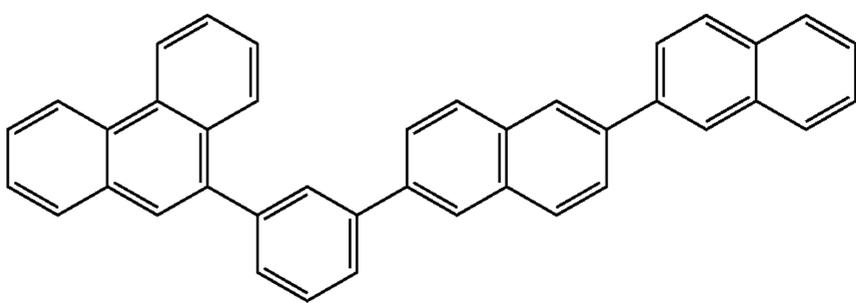
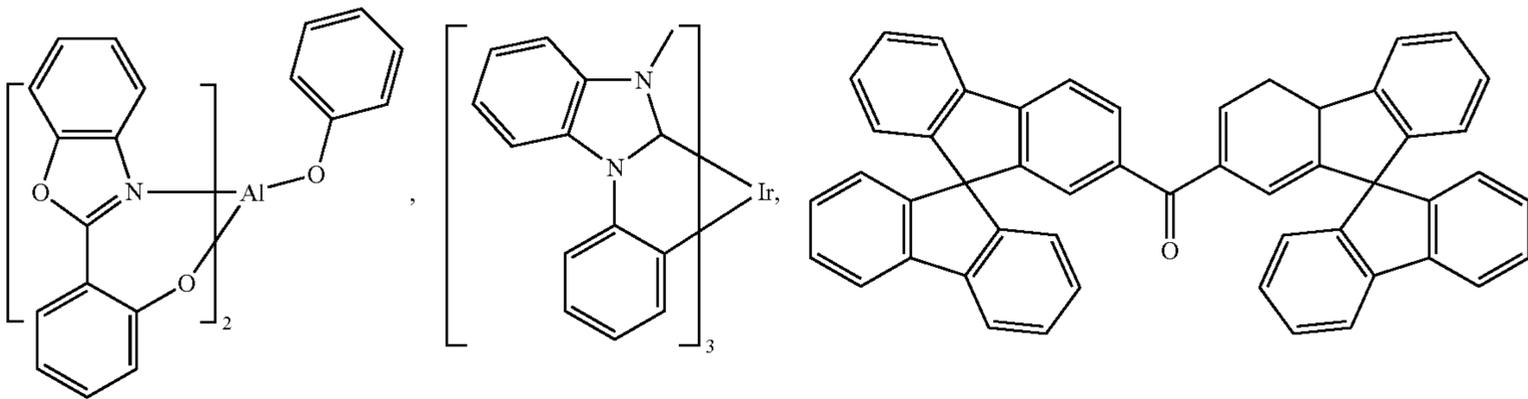
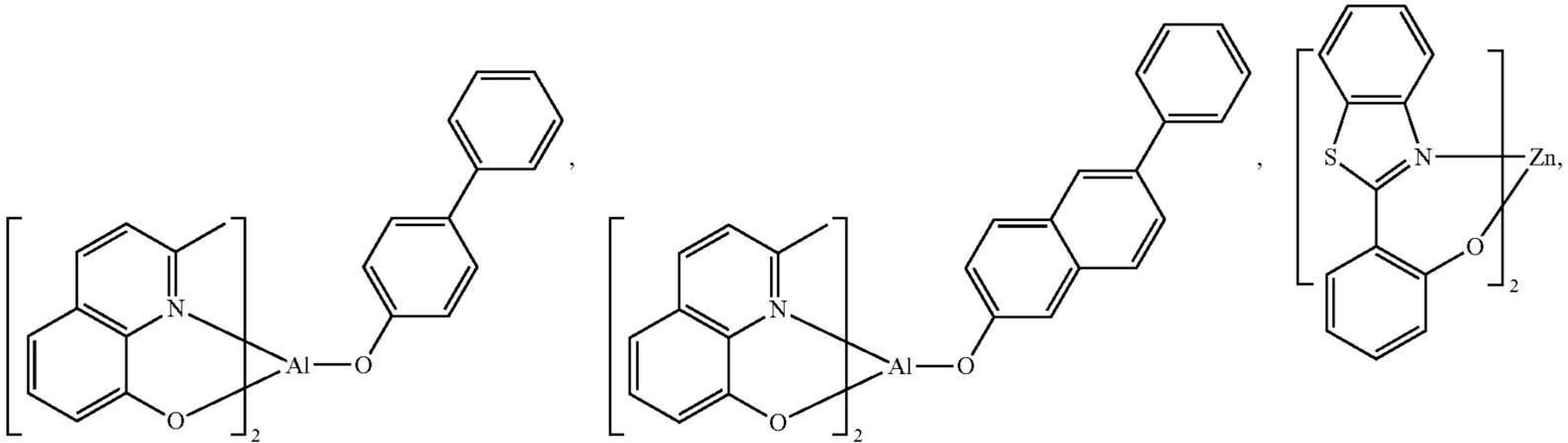
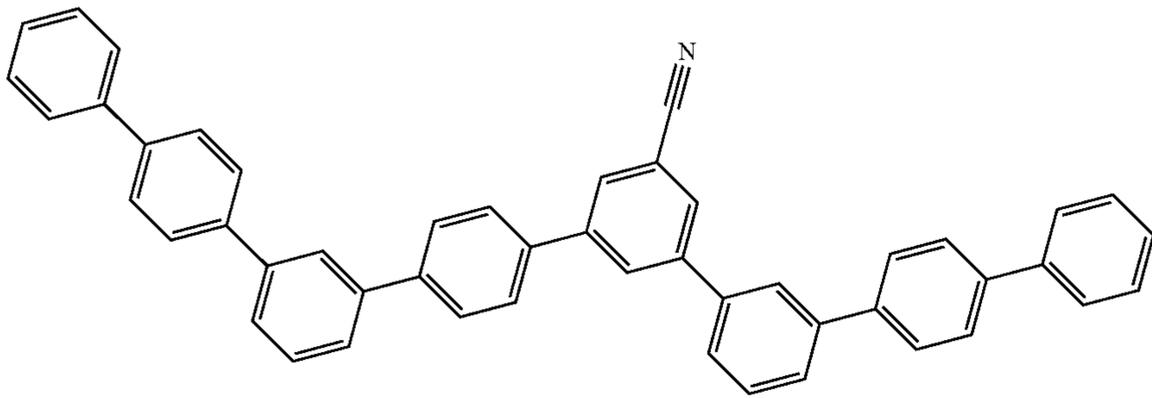
-continued



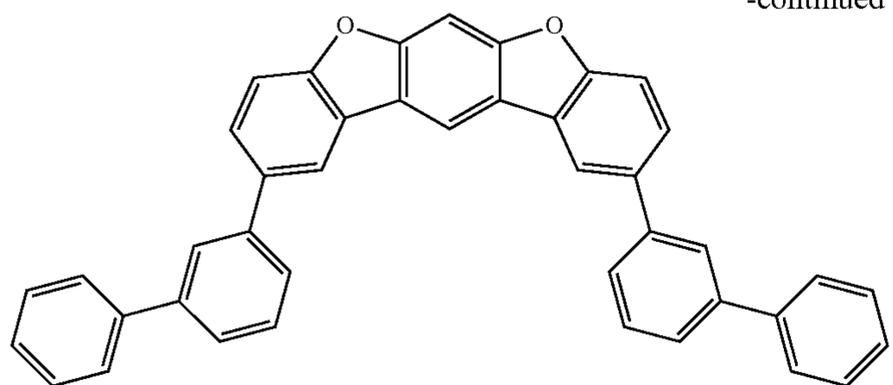
-continued



-continued



123



-continued

124

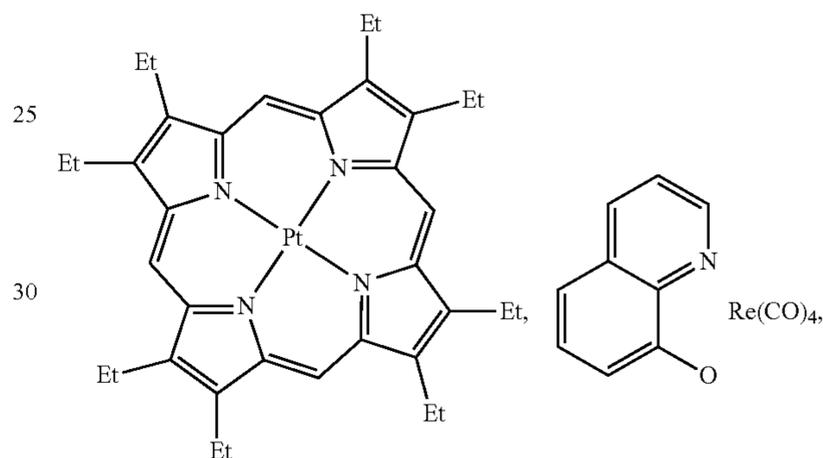
Emitter:

An emitter example is not particularly limited, and any compound may be used as long as the compound is typically used as an emitter material. Examples of suitable emitter materials include, but are not limited to, compounds which can produce emissions via phosphorescence, fluorescence, thermally activated delayed fluorescence, i.e., TADF (also referred to as E-type delayed fluorescence), triplet-triplet annihilation, or combinations of these processes.

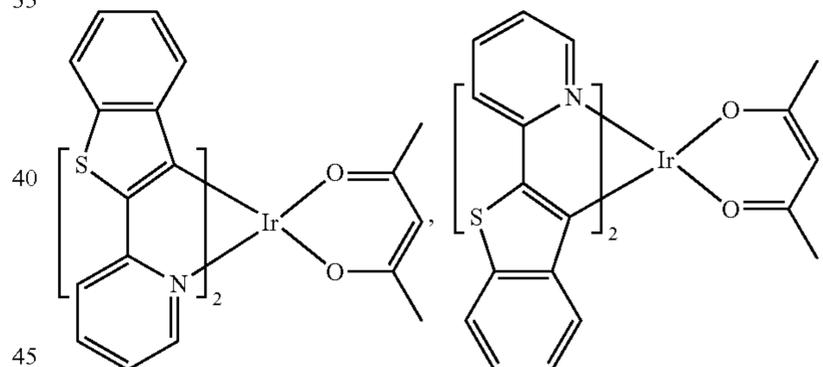
Non-limiting examples of the emitter materials that may be used in an OLED in combination with materials disclosed herein are exemplified below together with references that disclose those materials: CN103694277, CN1696137, EB01238981, EP01239526, EP01961743, EP1239526, EP1244155, EP1642951, EP1647554, EP1841834, EP1841834B, EP2062907, EP2730583, JP2012074444, JP2013110263, JP4478555, KR1020090133652, KR20120032054, KR20130043460, TW201332980, U.S. Ser. No. 06/699,599, U.S. Ser. No. 06/916,554, US20010019782, US20020034656, US20030068526, US20030072964, US20030138657, US20050123788, US20050244673, US2005123791, US2005260449, US20060008670, US20060065890, US20060127696, US20060134459, US20060134462, US20060202194, US20060251923, US20070034863, US20070087321, US20070103060, US20070111026, US20070190359, US20070231600, US2007034863, US2007104979, US2007104980, US2007138437, US2007224450, US2007278936, US20080020237, US20080233410, US20080261076, US20080297033, US200805851, US2008161567, US2008210930, US20090039776, US20090108737, US20090115322, US20090179555, US2009085476, US2009104472, US20100090591, US20100148663, US20100244004, US20100295032, US2010102716, US2010105902, US2010244004, US2010270916, US20110057559, US20110108822, US20110204333, US2011215710, US2011227049, US2011285275, US2012292601, US20130146848, US2013033172, US2013165653, US2013181190, US2013334521, US20140246656, US2014103305, U.S. Pat. Nos. 6,303,238, 6,413,656, 6,653,654, 6,670,645, 6,687,266, 6,835,469, 6,921,915, 7,279,704, 7,332,232, 7,378,162, 7,534,505, 7,675,228, 7,728,137, 7,740,957, 7,759,489, 7,951,947, 8,067,099, 8,592,586, 8,871,361, WO06081973, WO06121811, WO07018067, WO07108362, WO07115970, WO07115981, WO08035571, WO2002015645, WO2003040257, WO2005019373, WO2006056418, WO2008054584, WO2008078800, WO2008096609, WO2008101842, WO2009000673, WO2009050281, WO2009100991, WO2010028151, WO2010054731, WO2010086089, WO2010118029, WO2011044988, WO2011051404,

15 WO2011107491, WO2012020327, WO2012163471,  
 WO2013094620, WO2013107487, WO2013174471,  
 WO2014007565, WO2014008982, WO2014023377,  
 WO2014024131, WO2014031977, WO2014038456,  
 WO2014112450,

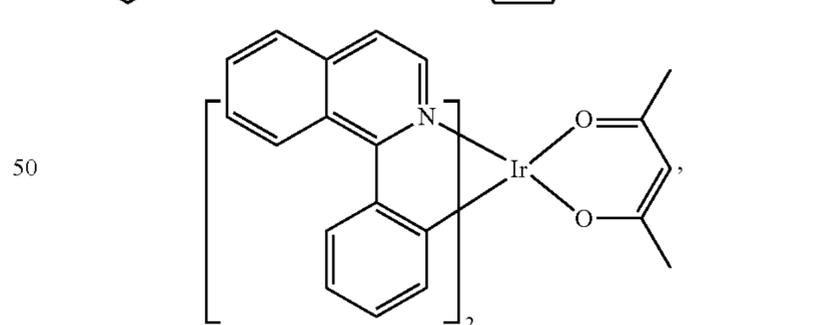
20



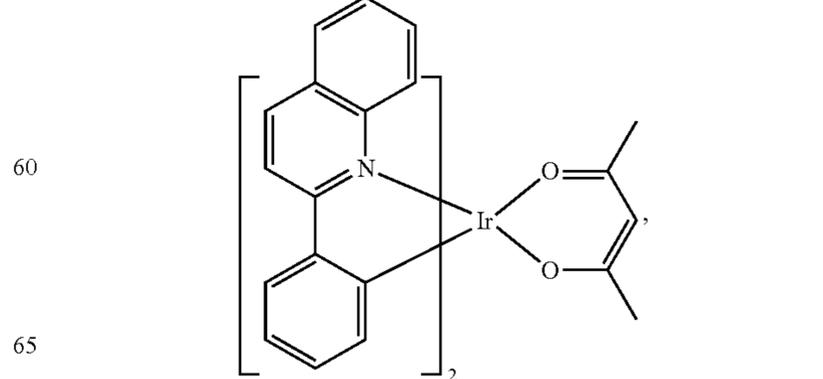
25



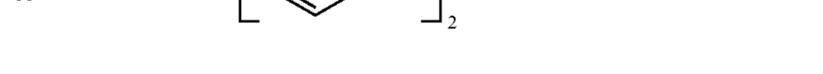
30



35



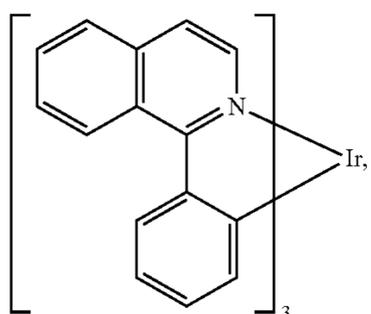
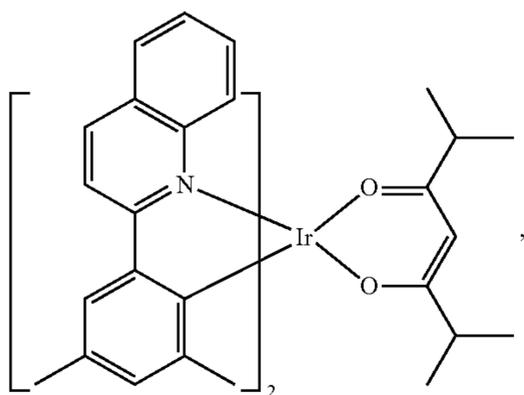
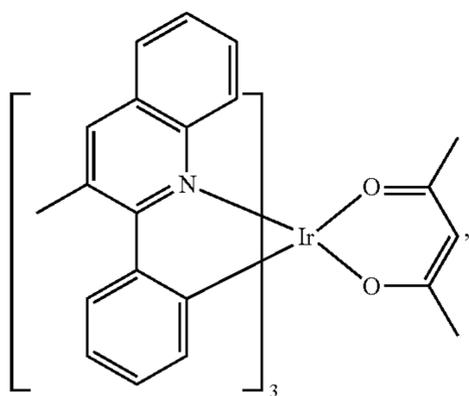
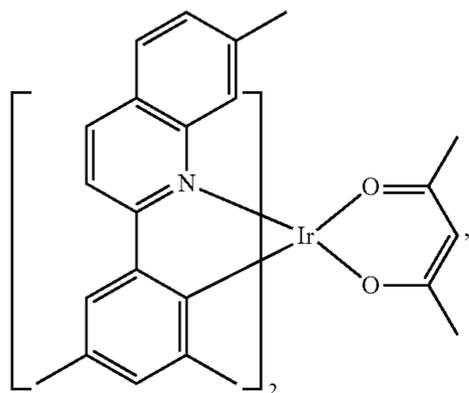
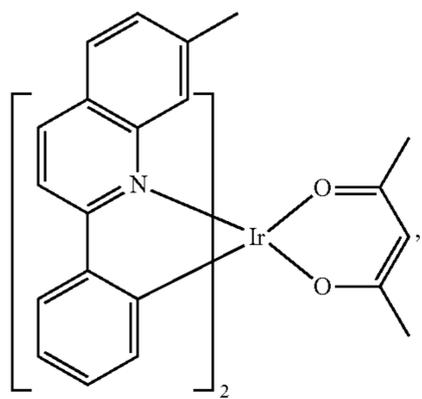
40



45

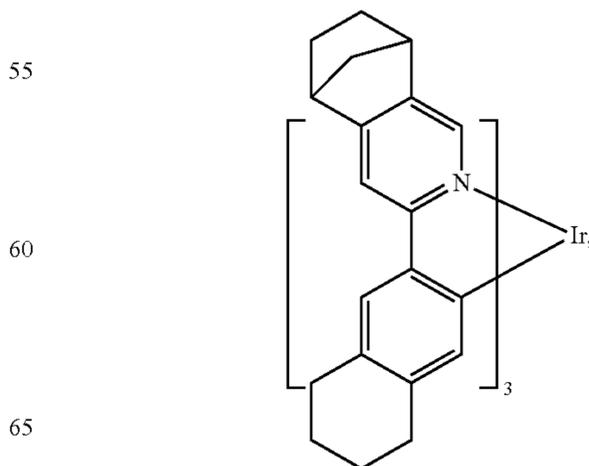
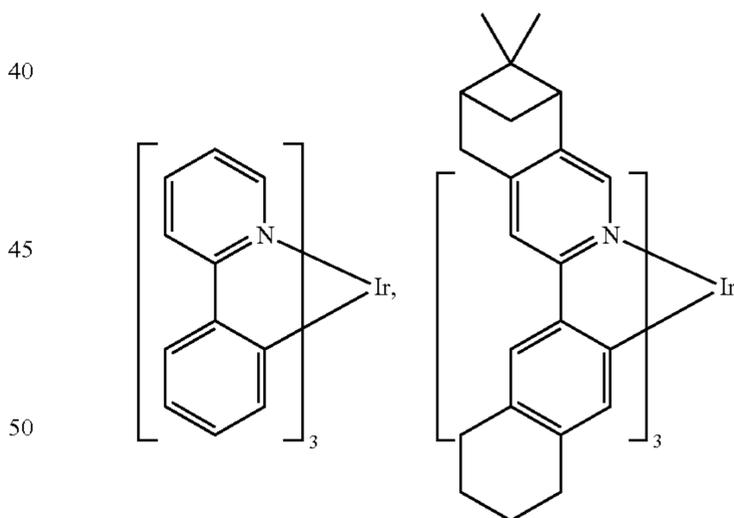
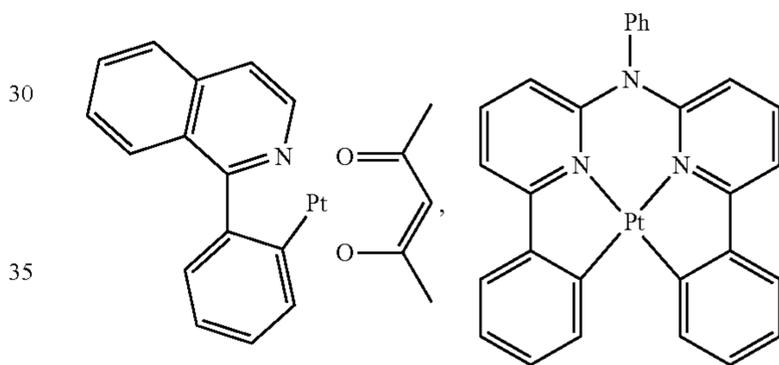
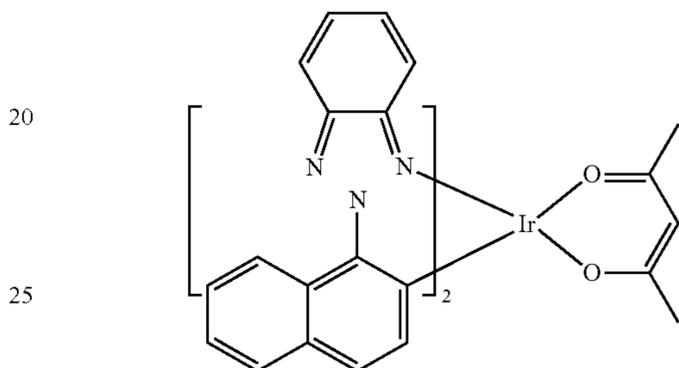
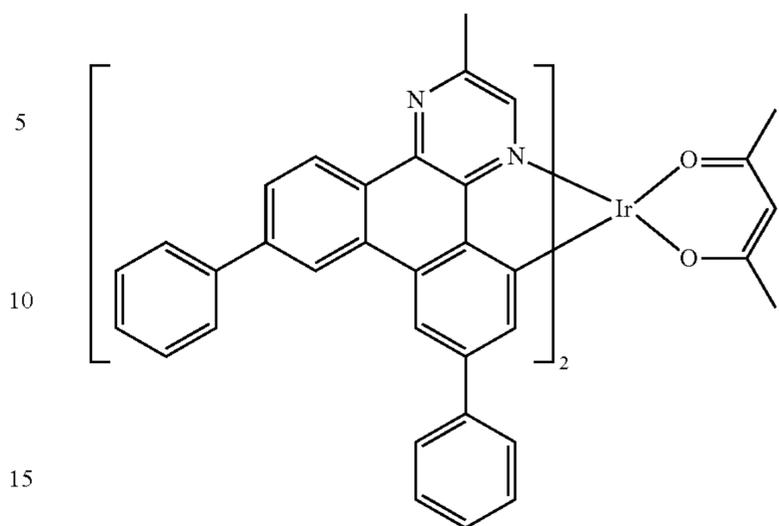
125

-continued



126

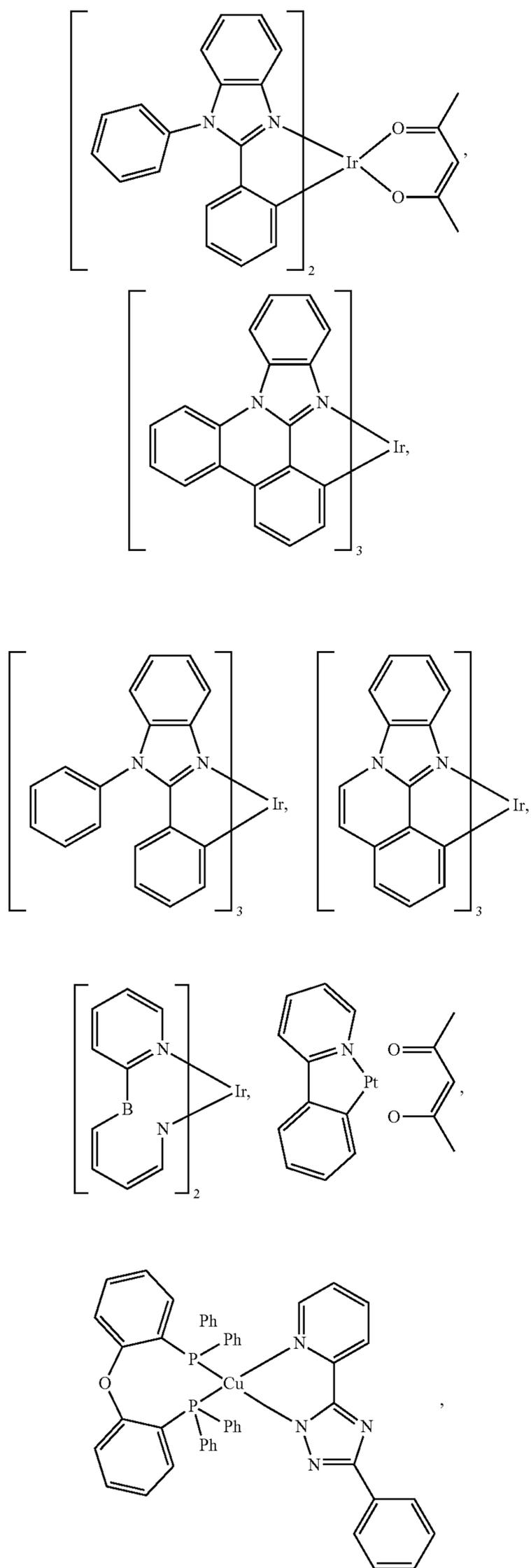
-continued





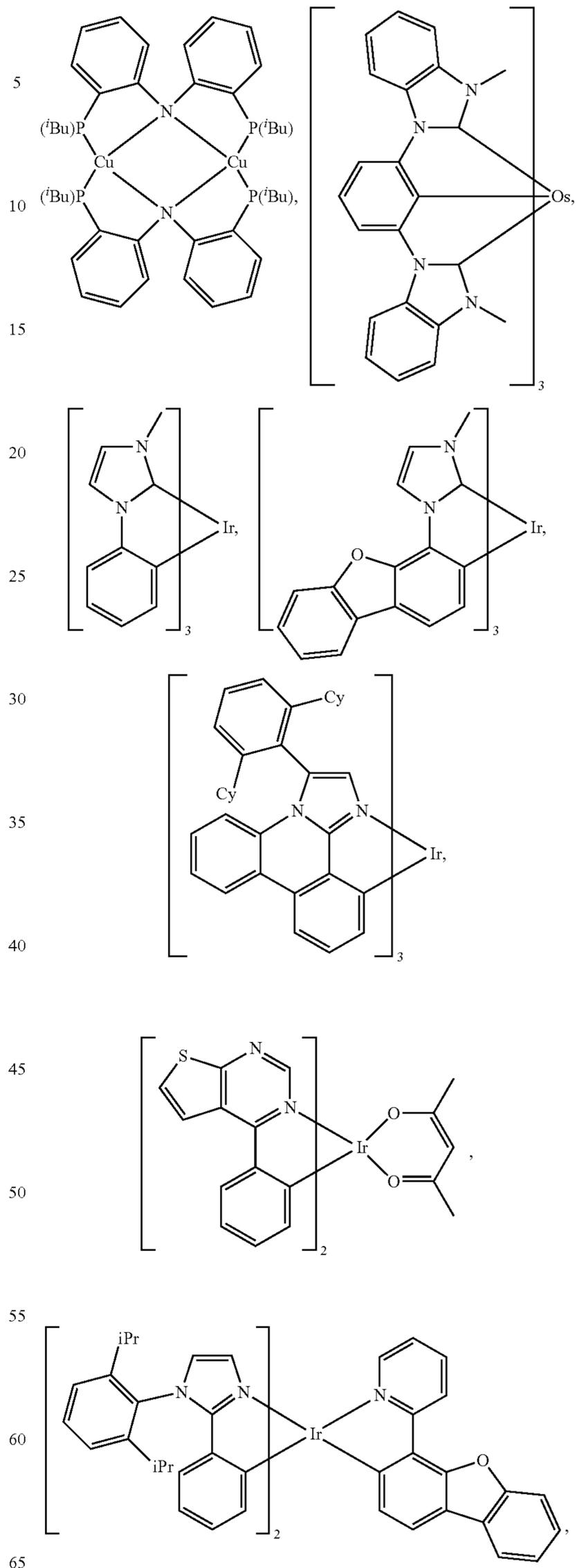
129

-continued



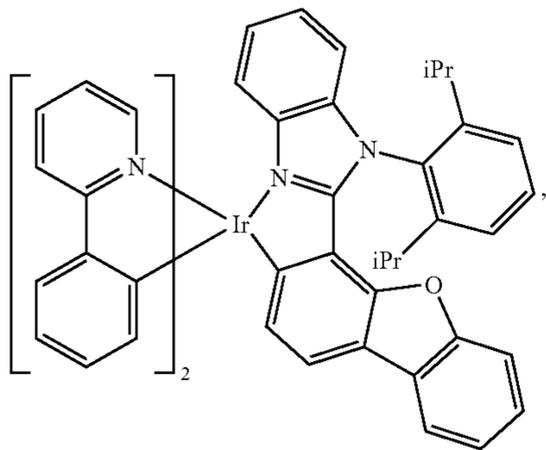
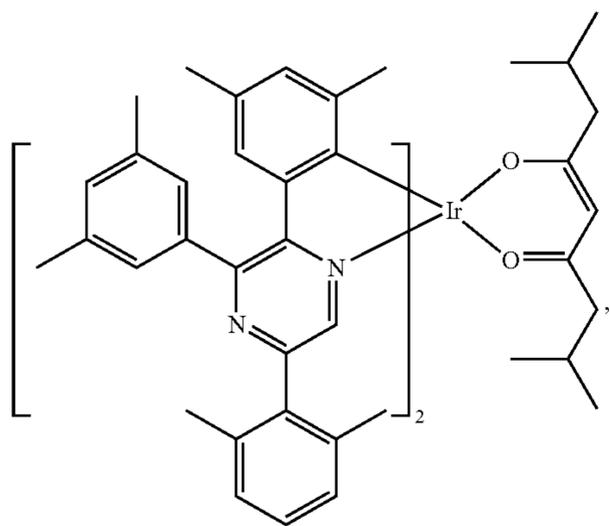
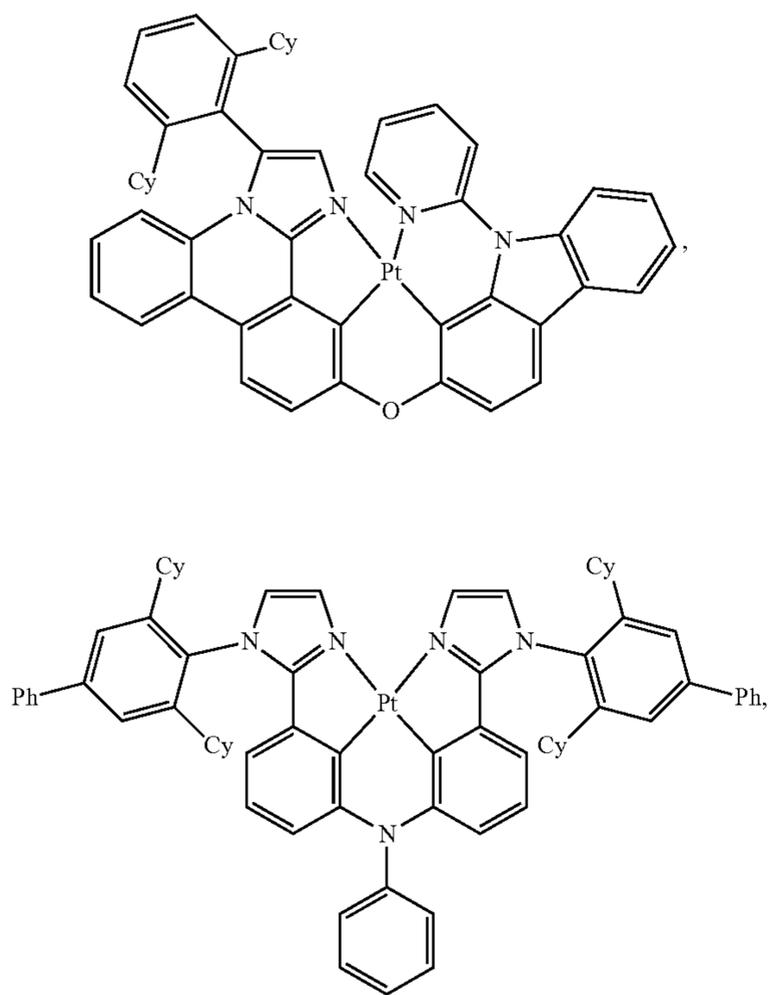
130

-continued



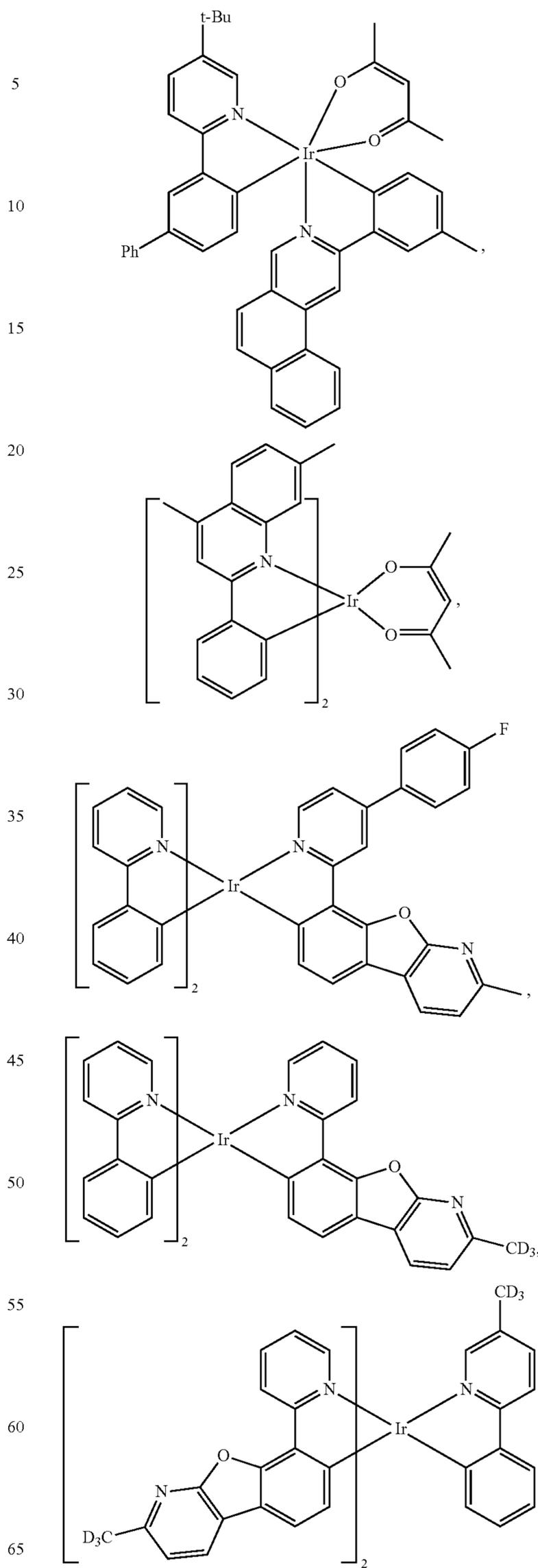
**131**

-continued



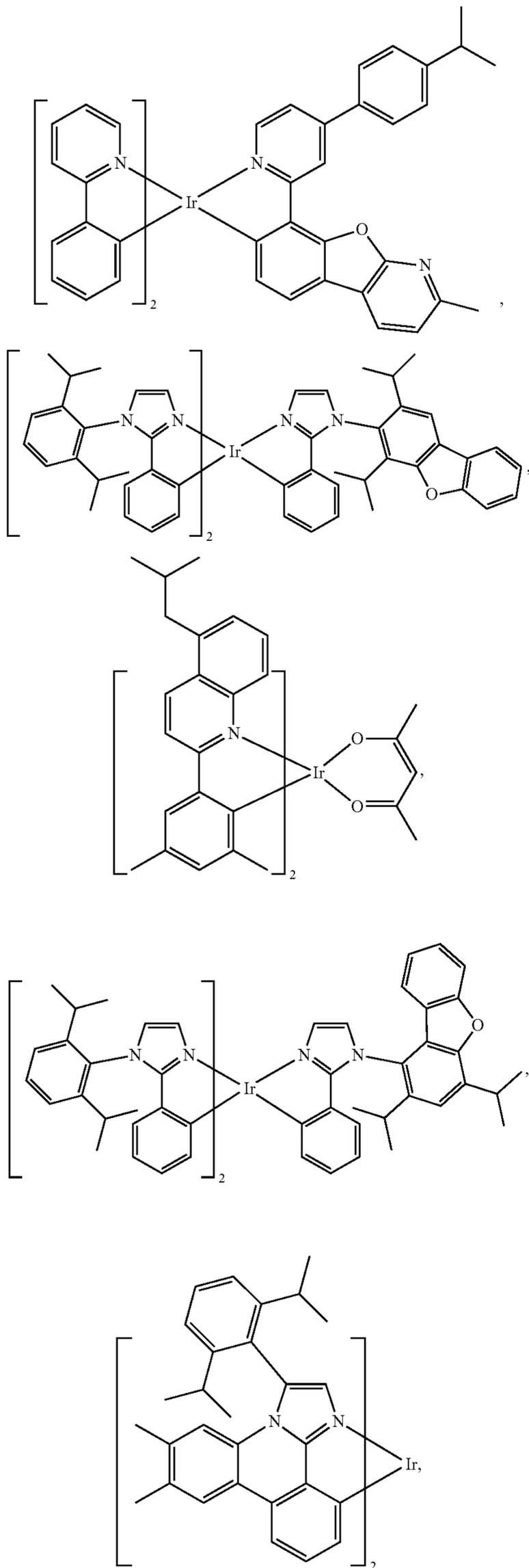
**132**

-continued



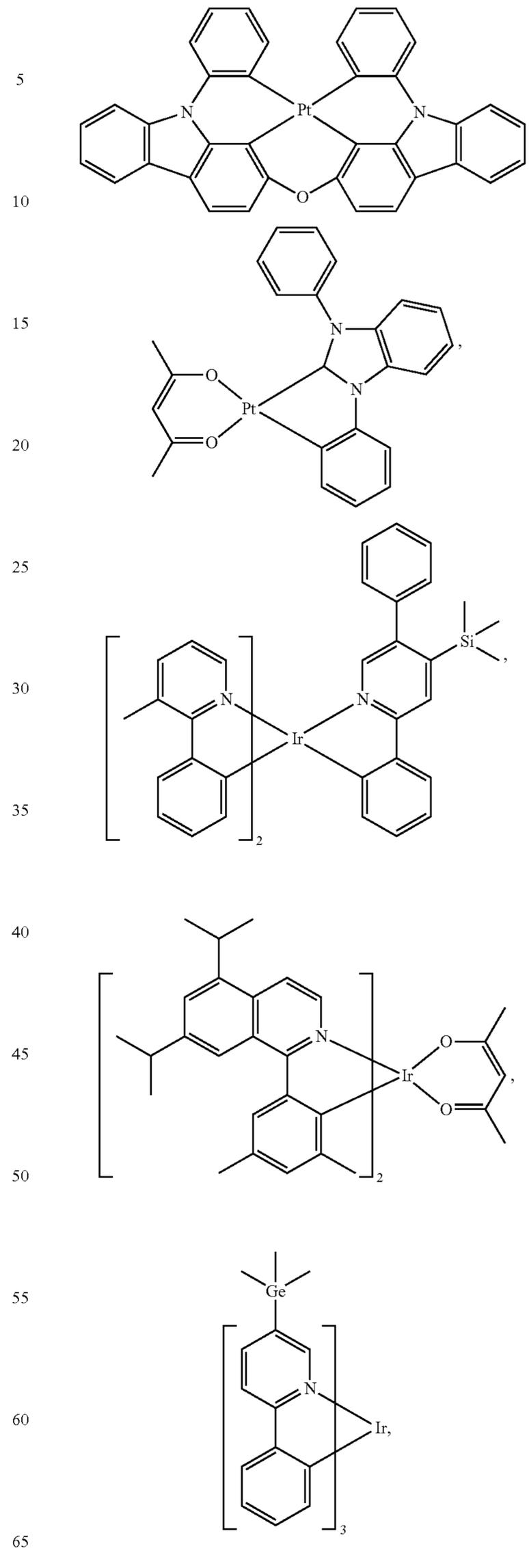
133

-continued



134

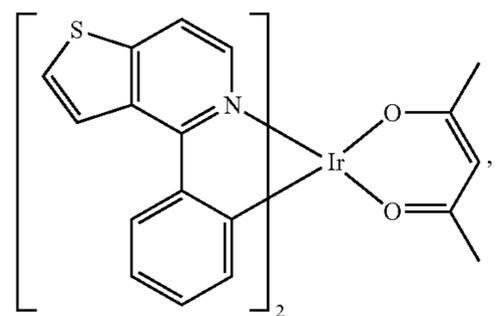
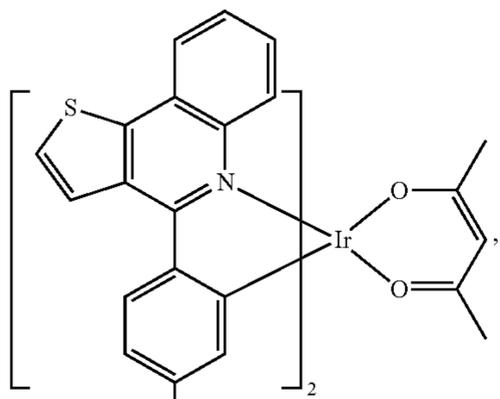
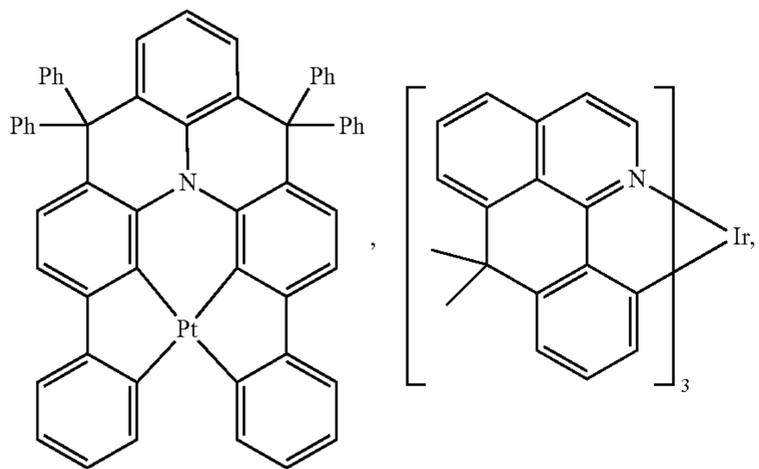
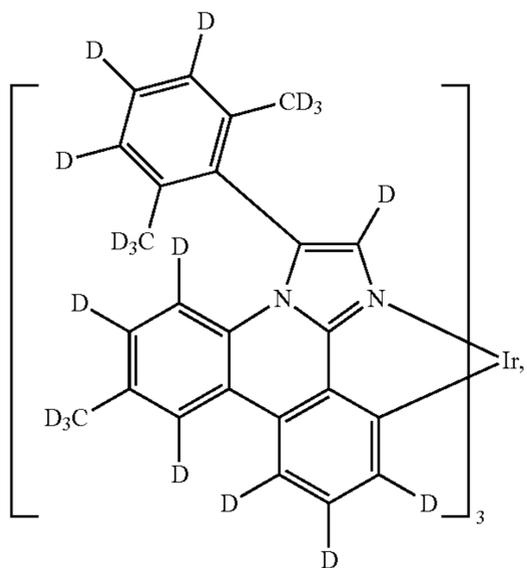
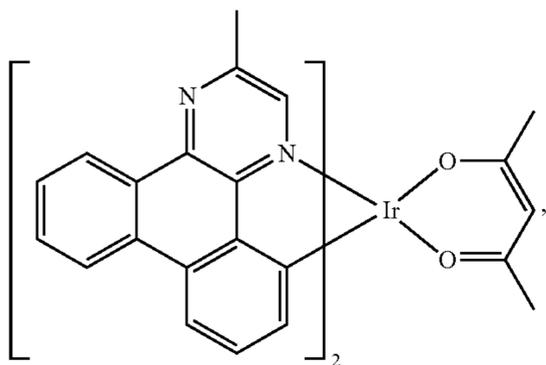
-continued



5  
10  
15  
20  
25  
30  
35  
40  
45  
50  
55  
60  
65

135

-continued



136

-continued

5

10

15

20

25

30

35

40

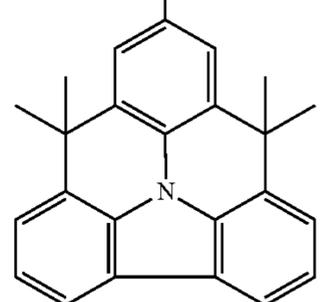
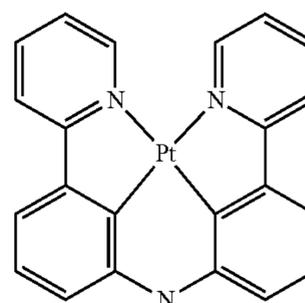
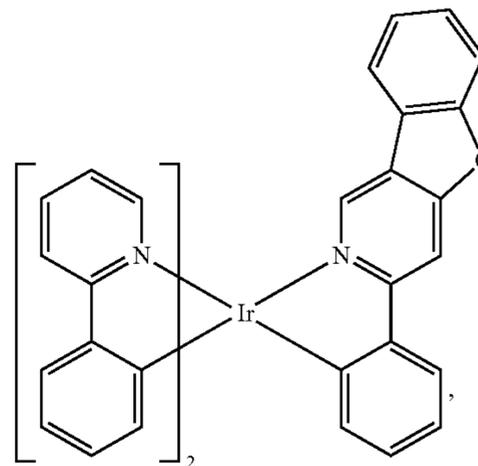
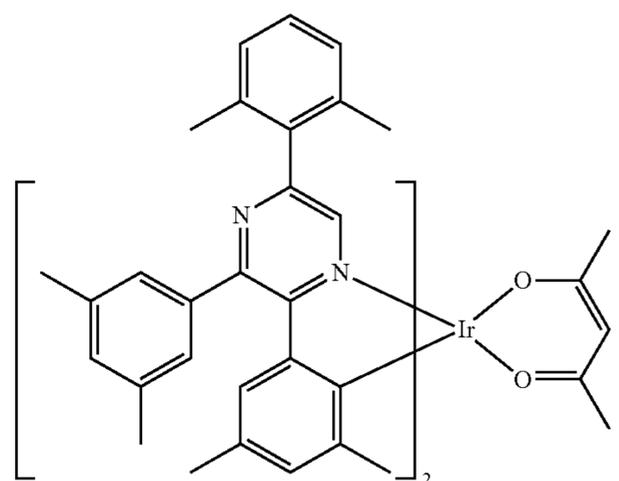
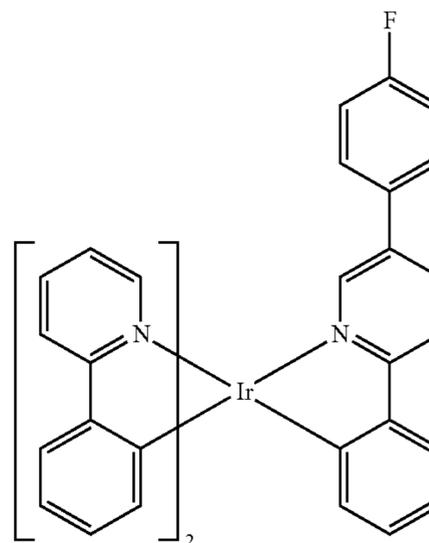
45

50

55

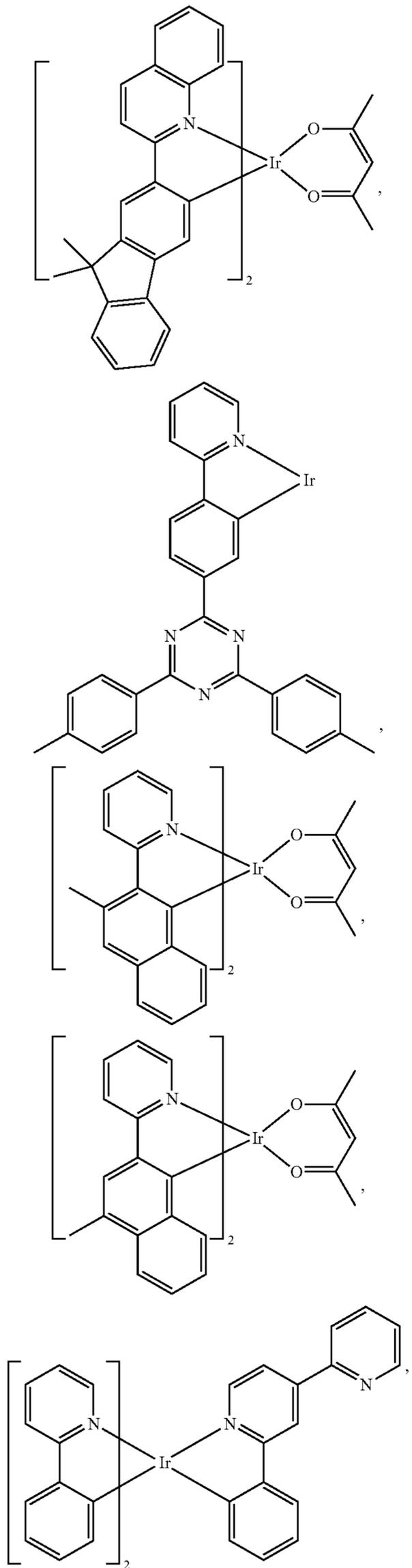
60

65



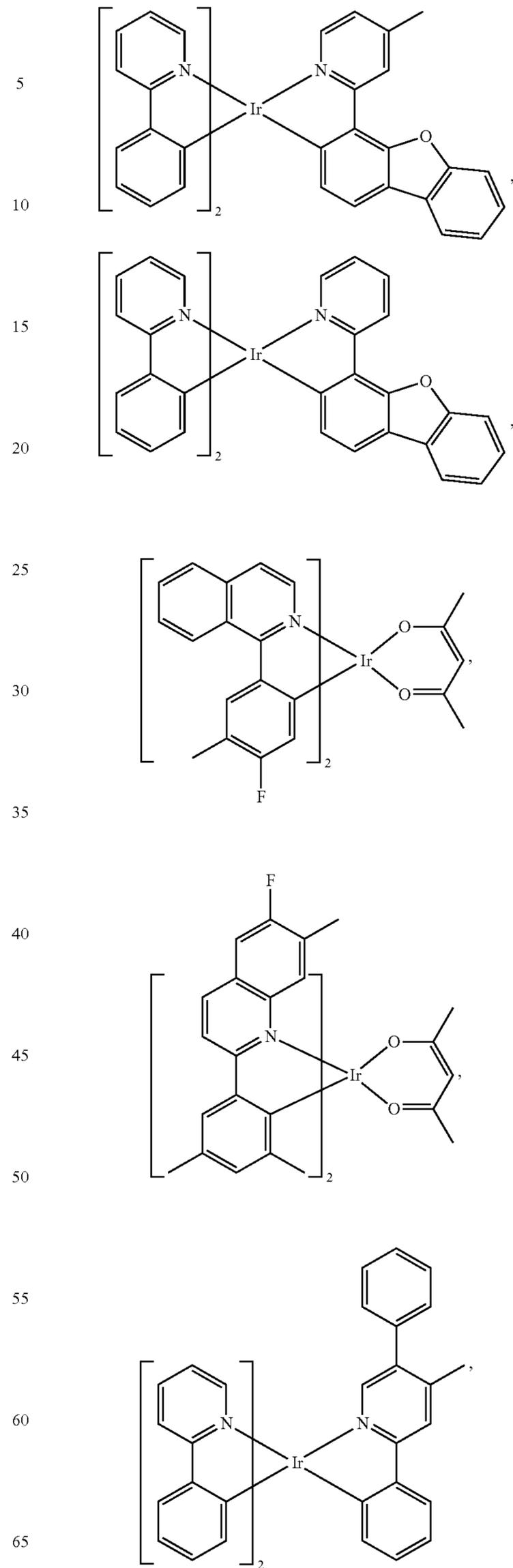
137

-continued



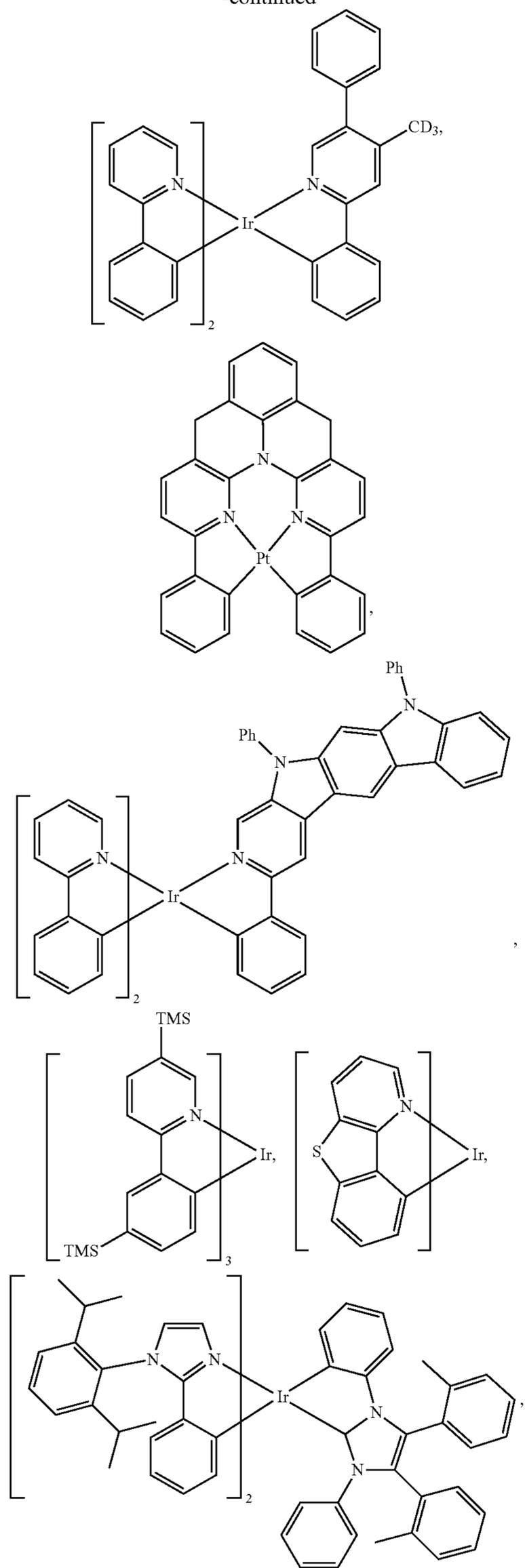
138

-continued



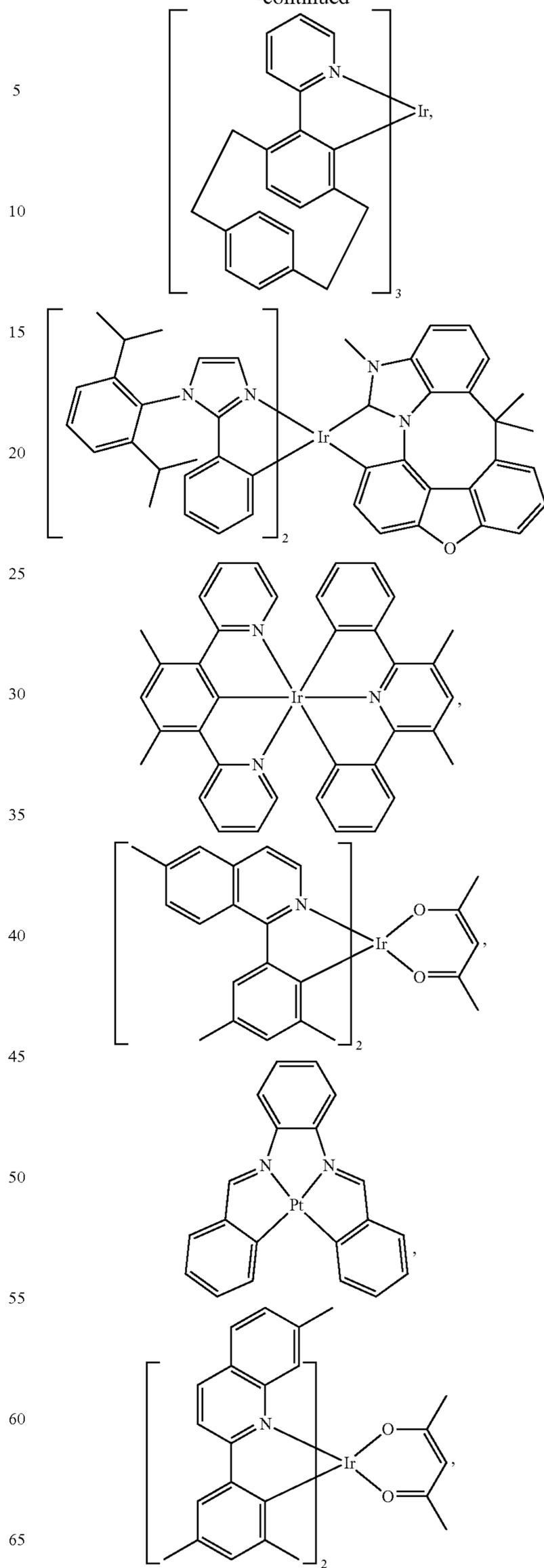
139

-continued



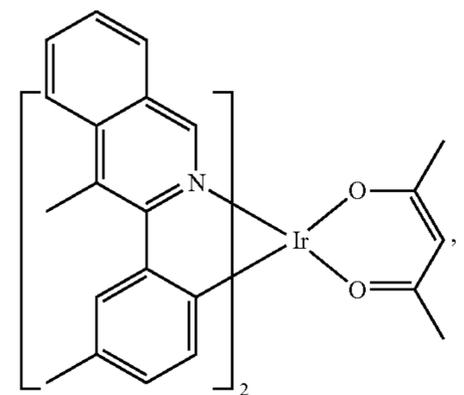
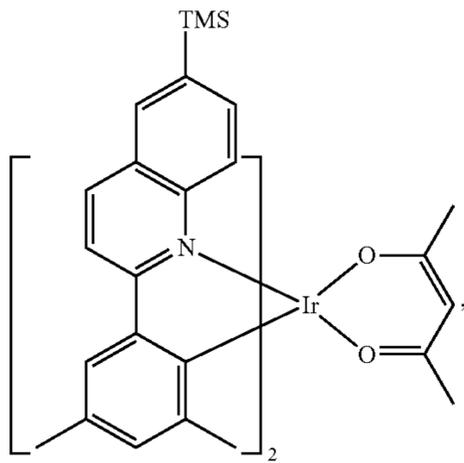
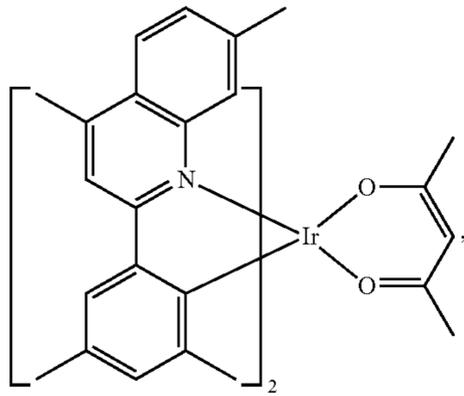
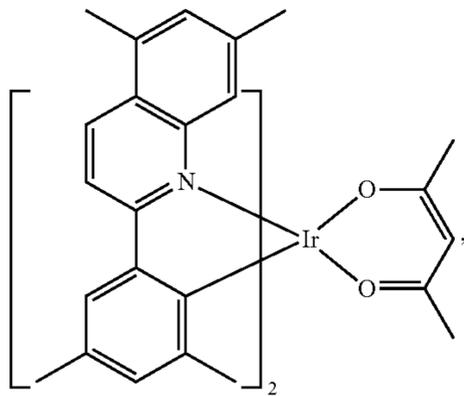
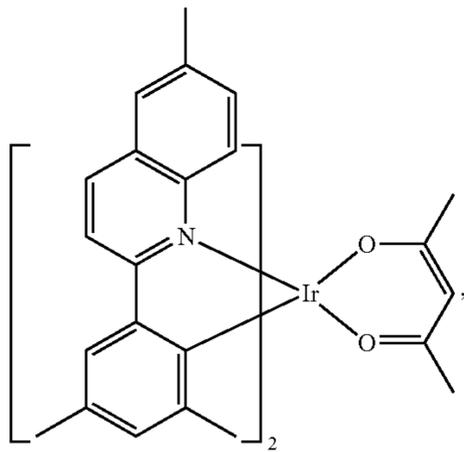
140

-continued



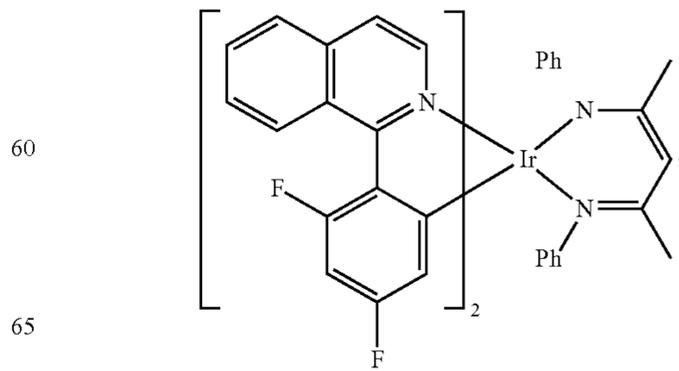
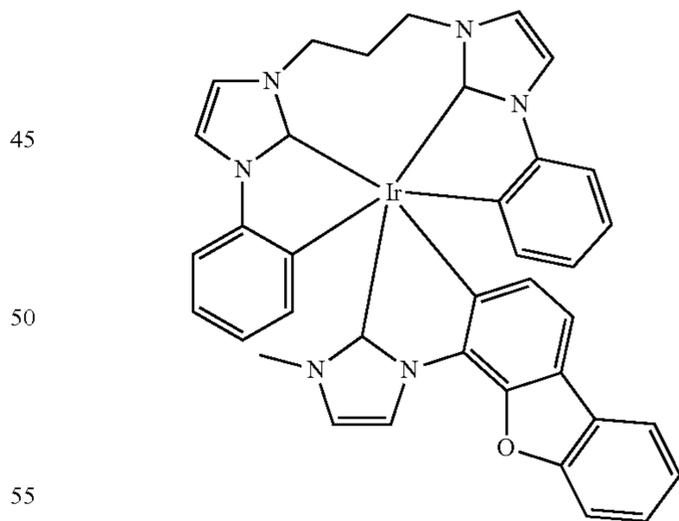
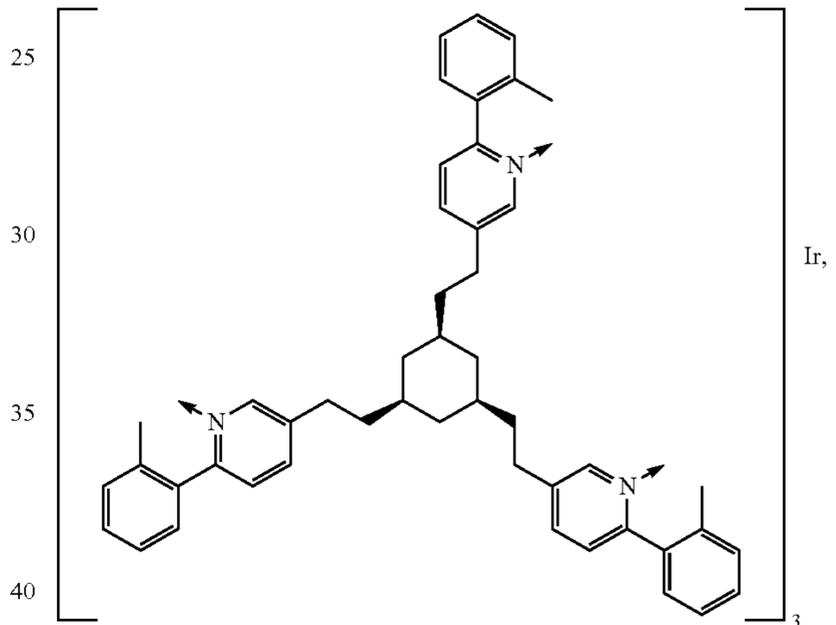
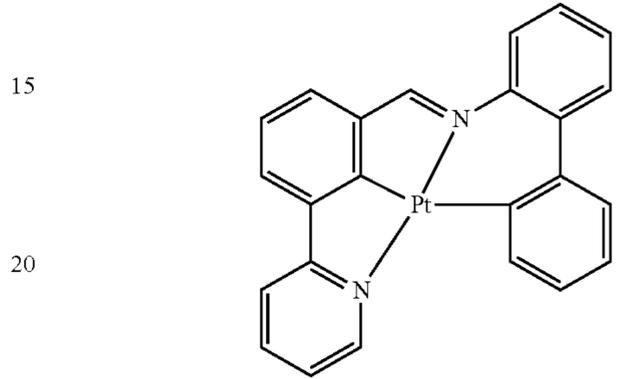
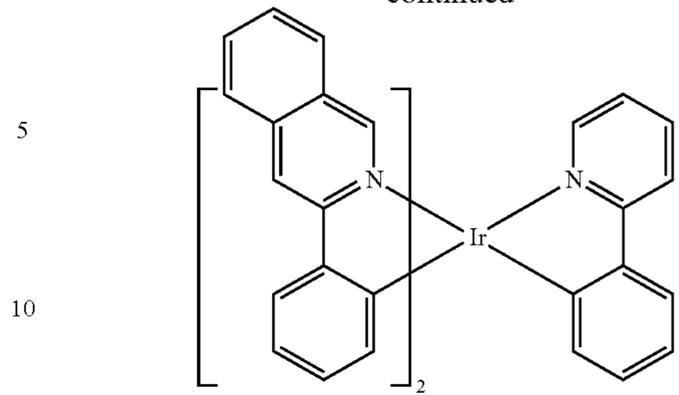
141

-continued



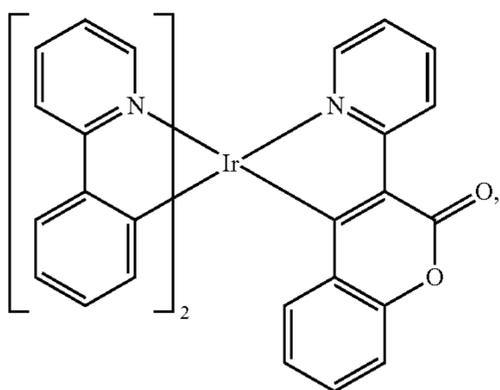
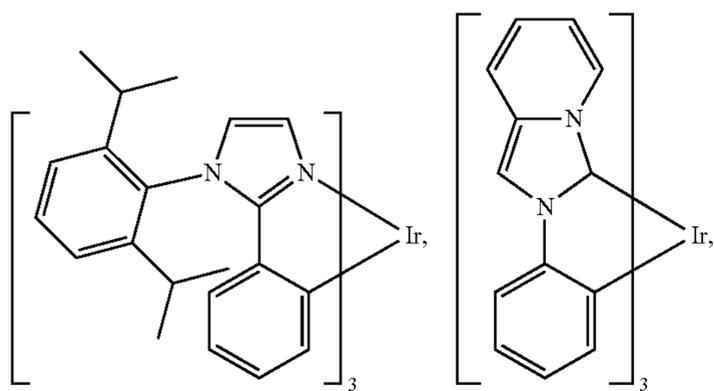
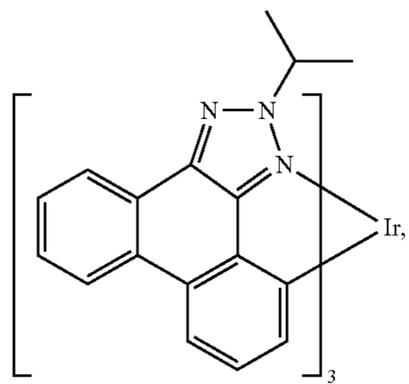
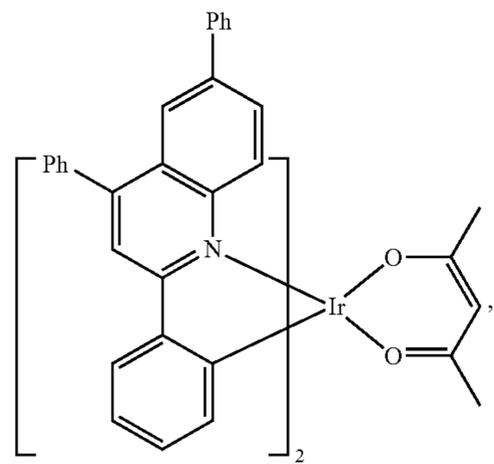
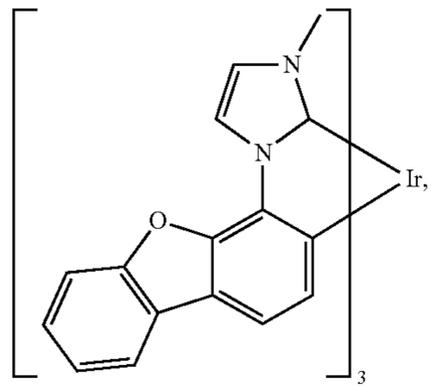
142

-continued



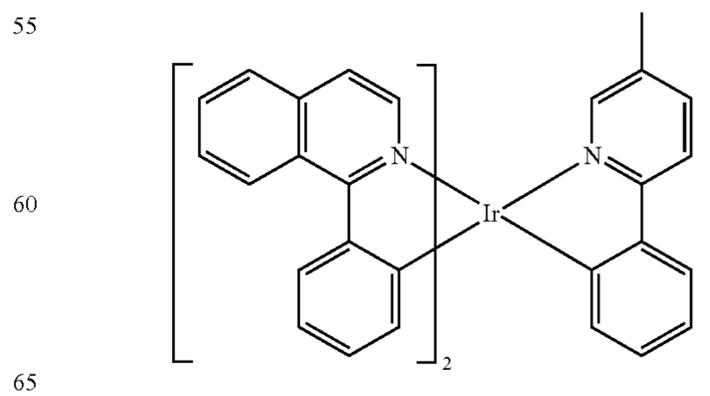
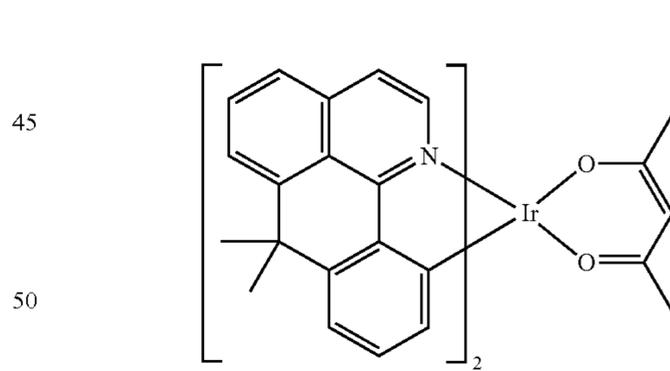
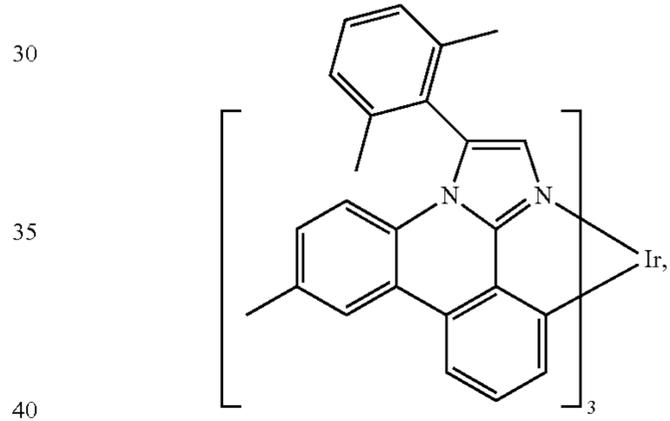
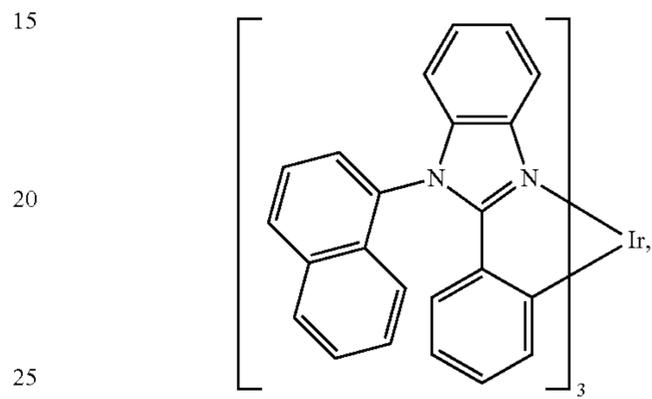
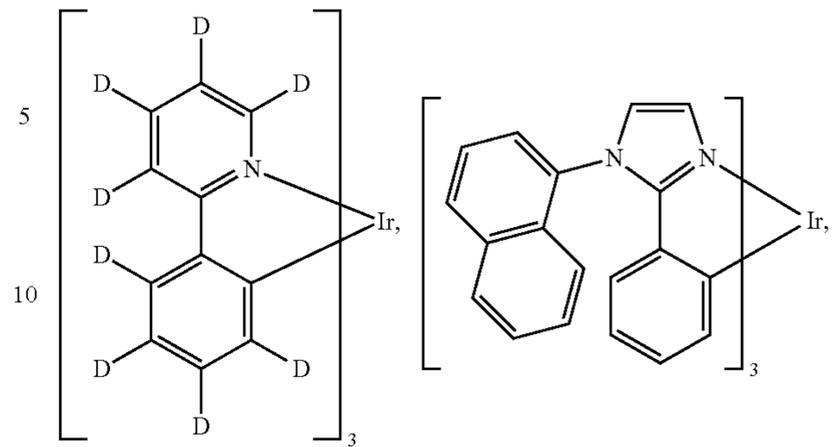
143

-continued



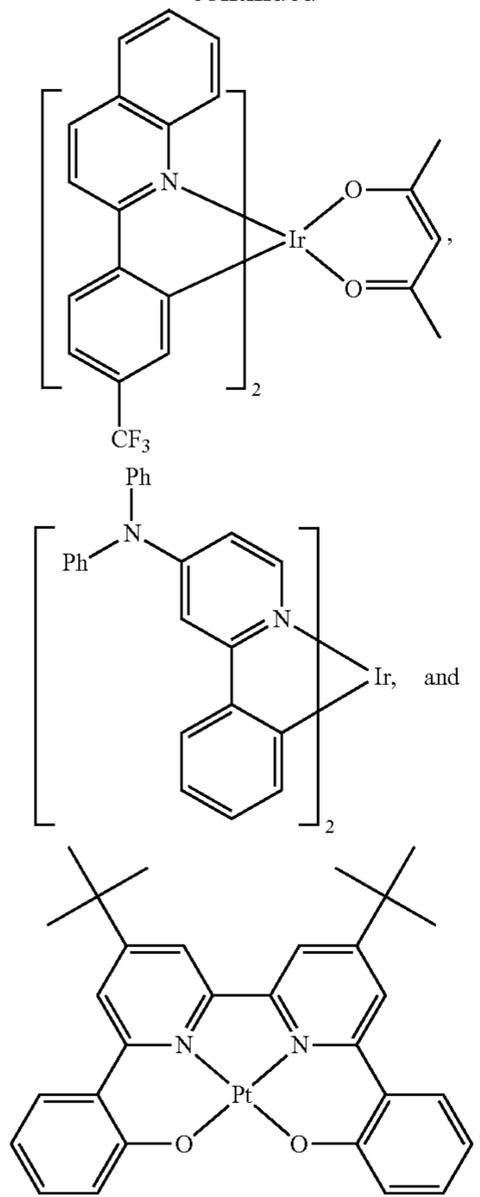
144

-continued



145

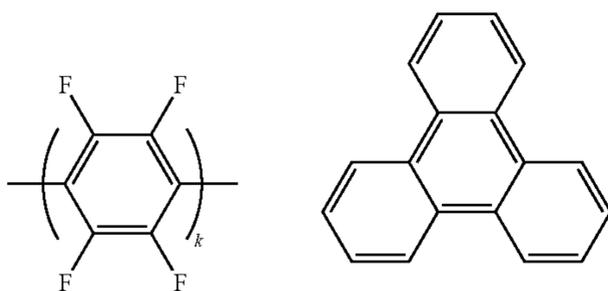
-continued



A hole blocking layer (HBL) may be used to reduce the number of holes and/or excitons that leave the emissive layer. The presence of such a blocking layer in a device may result in substantially higher efficiencies and/or longer lifetime as compared to a similar device lacking a blocking layer. Also, a blocking layer may be used to confine emission to a desired region of an OLED. In some embodiments, the HBL material has a lower HOMO (further from the vacuum level) and/or higher triplet energy than the emitter closest to the HBL interface. In some embodiments, the HBL material has a lower HOMO (further from the vacuum level) and/or higher triplet energy than one or more of the hosts closest to the HBL interface.

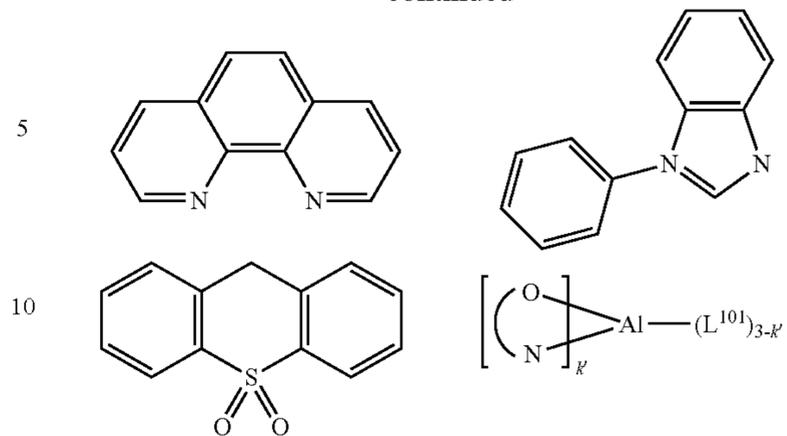
In one aspect, compound used in HBL contains the same molecule or the same functional groups used as host described above.

In another aspect, compound used in HBL contains at least one of the following groups in the molecule:



146

-continued

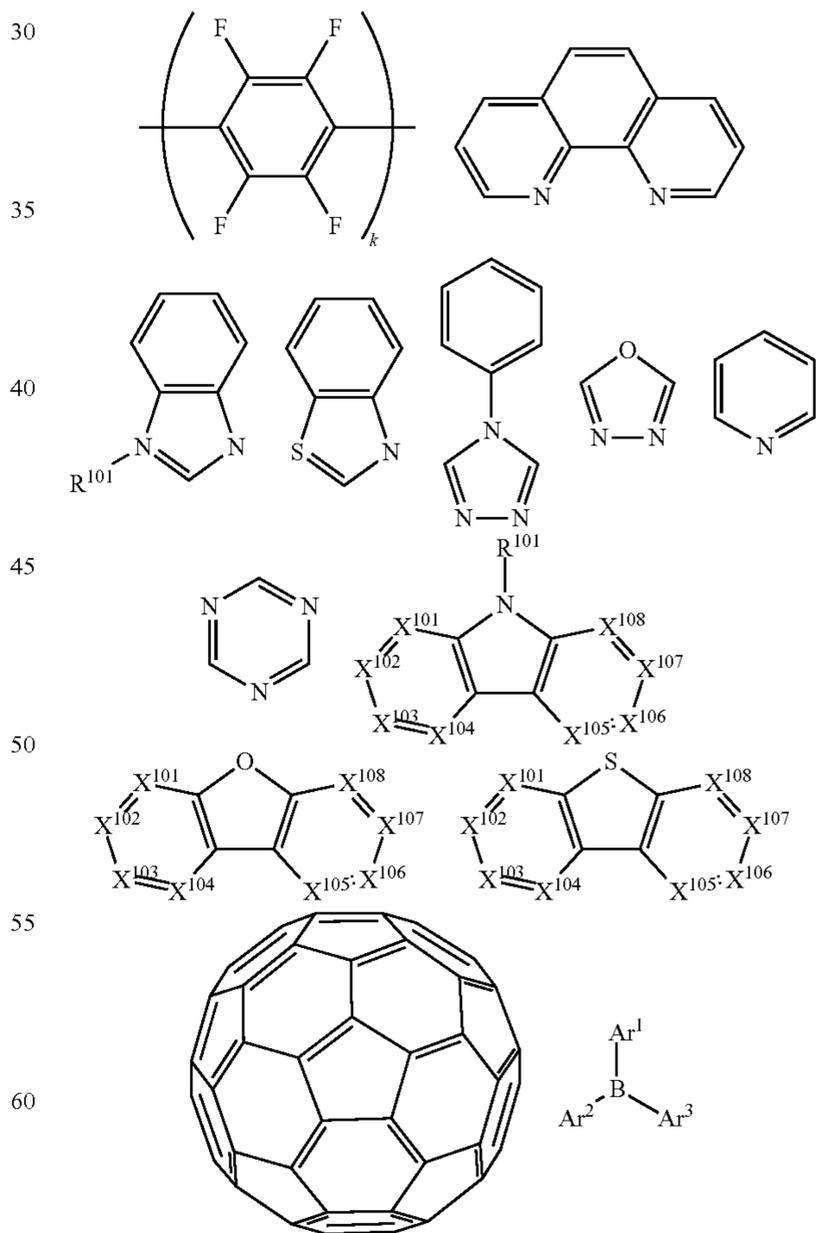


wherein  $k$  is an integer from 1 to 20;  $L^{101}$  is an another ligand,  $k'$  is an integer from 1 to 3.

ETL:

Electron transport layer (ETL) may include a material capable of transporting electrons. Electron transport layer may be intrinsic (undoped), or doped. Doping may be used to enhance conductivity. Examples of the ETL material are not particularly limited, and any metal complexes or organic compounds may be used as long as they are typically used to transport electrons.

In one aspect, compound used in ETL contains at least one of the following groups in the molecule:

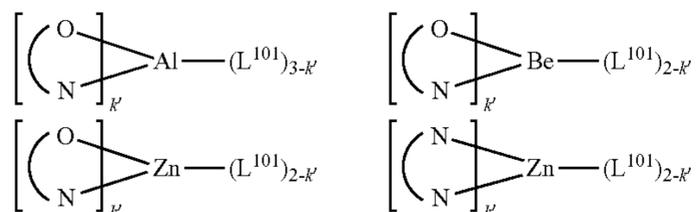


wherein  $R^{101}$  is selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, aryl-

147

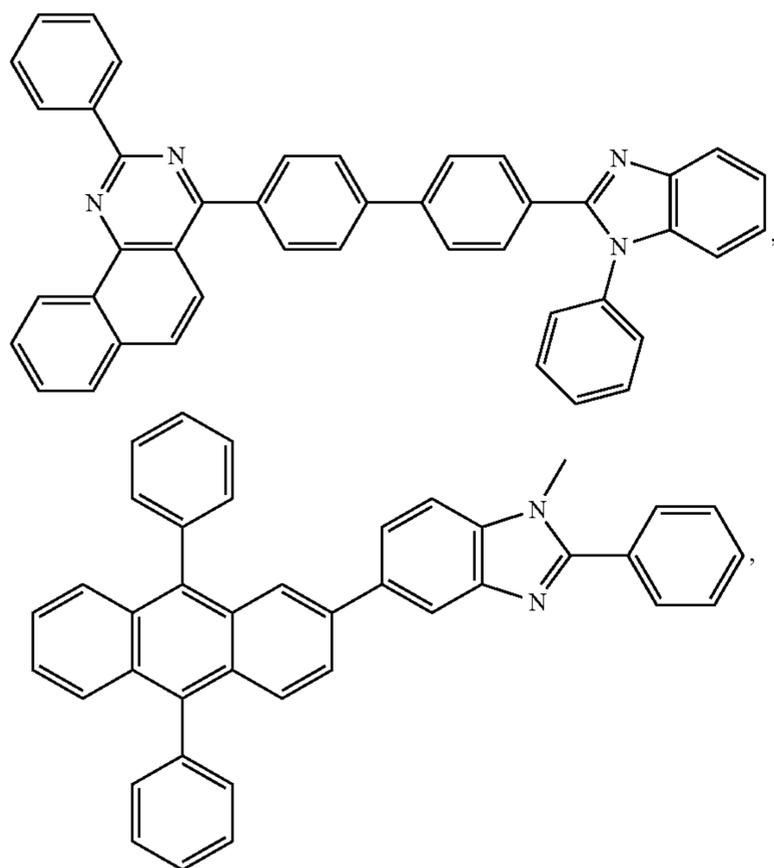
alkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof, when it is aryl or heteroaryl, it has the similar definition as Ar's mentioned above. Ar<sup>1</sup> to Ar<sup>3</sup> has the similar definition as Ar's mentioned above. k is an integer from 1 to 20. X<sup>101</sup> to X<sup>108</sup> is selected from C (including CH) or N.

In another aspect, the metal complexes used in ETL include, but are not limited to the following general formula:



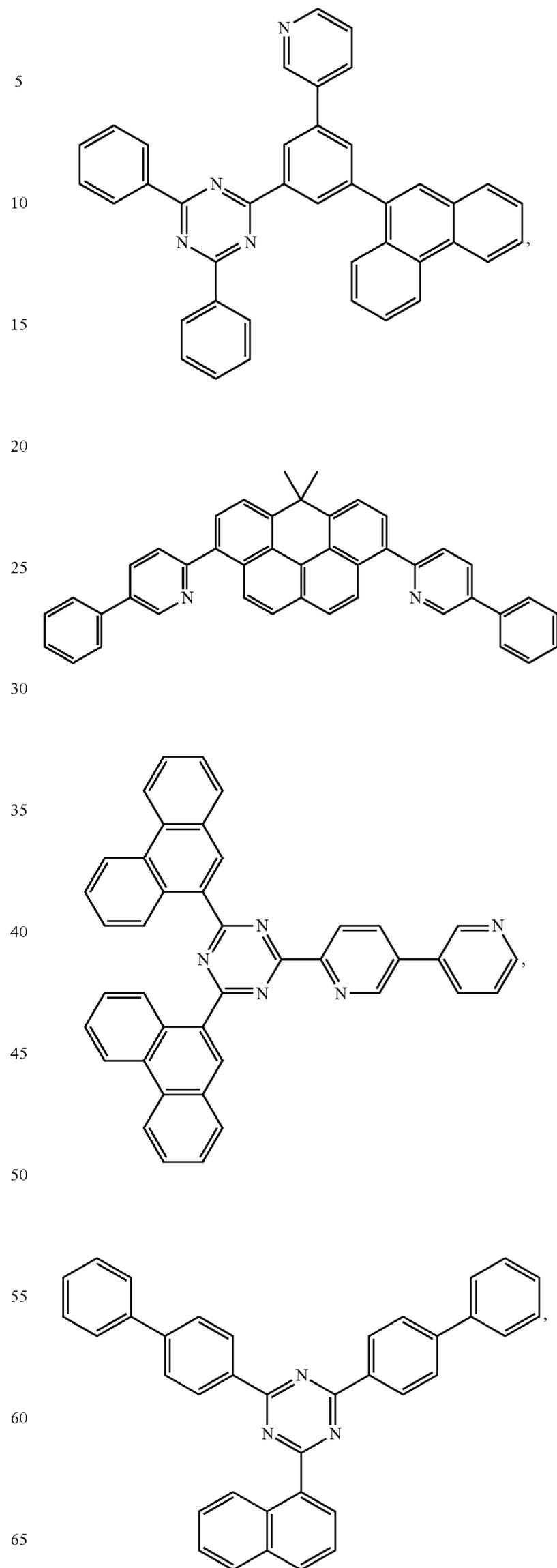
wherein (O—N) or (N—N) is a bidentate ligand, having metal coordinated to atoms O, N or N, N; L<sup>101</sup> is another ligand; k' is an integer value from 1 to the maximum number of ligands that may be attached to the metal.

Non-limiting examples of the ETL materials that may be used in an OLED in combination with materials disclosed herein are exemplified below together with references that disclose those materials: CN103508940, EP01602648, EP01734038, EP01956007, JP2004-022334, JP2005149918, JP2005-268199, KR0117693, KR20130108183, US20040036077, US20070104977, US2007018155, US20090101870, US20090115316, US20090140637, US20090179554, US2009218940, US2010108990, US2011156017, US2011210320, US2012193612, US2012214993, US2014014925, US2014014927, US20140284580, U.S. Pat. Nos. 6,656,612, 8,415,031, WO2003060956, WO2007111263, WO2009148269, WO2010067894, WO2010072300, WO2011074770, WO2011105373, WO2013079217, WO2013145667, WO2013180376, WO2014104499, WO2014104535,



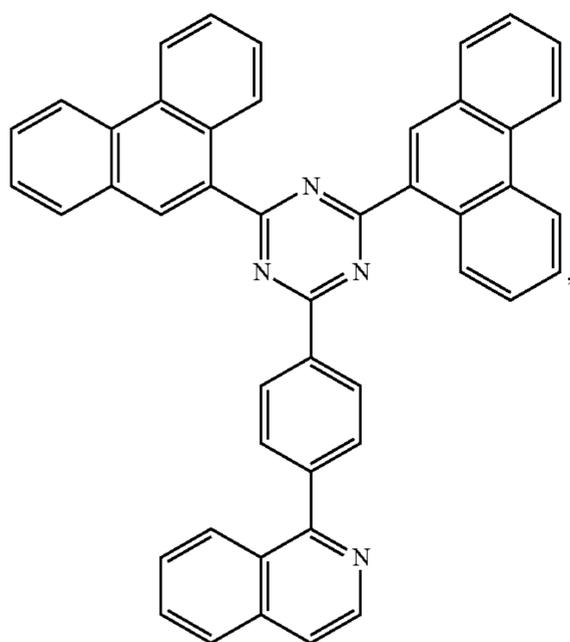
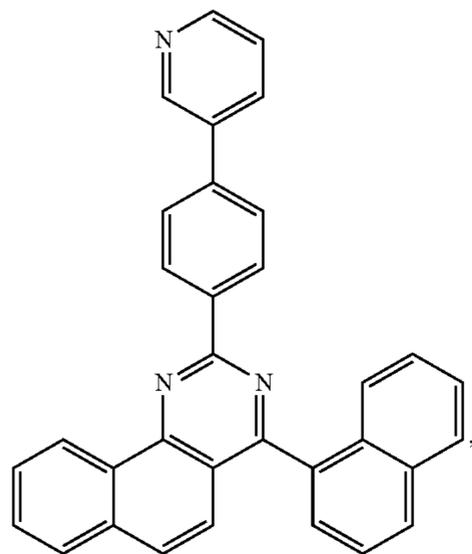
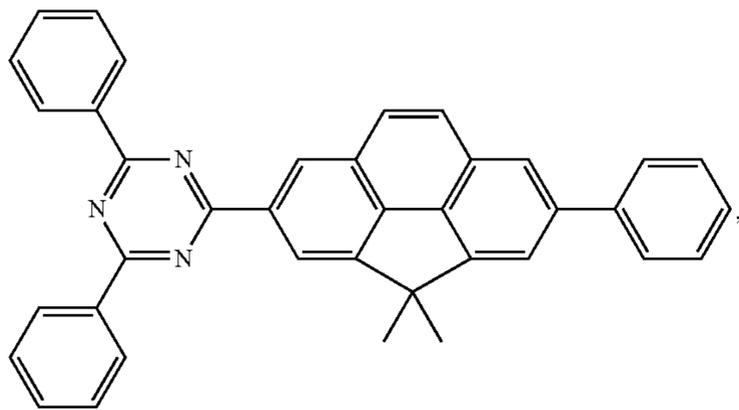
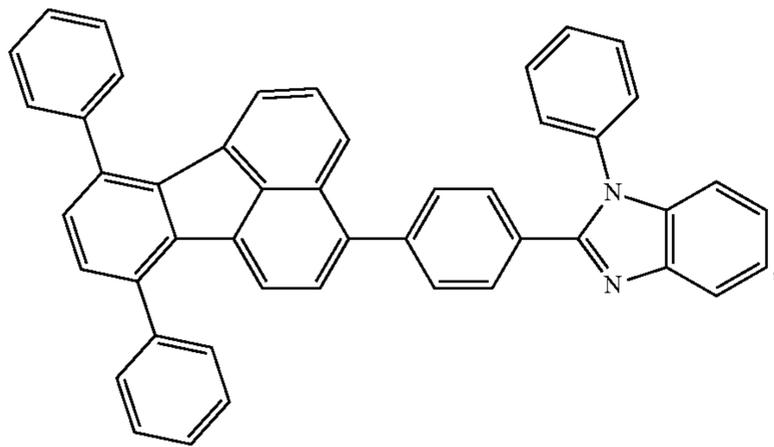
148

-continued



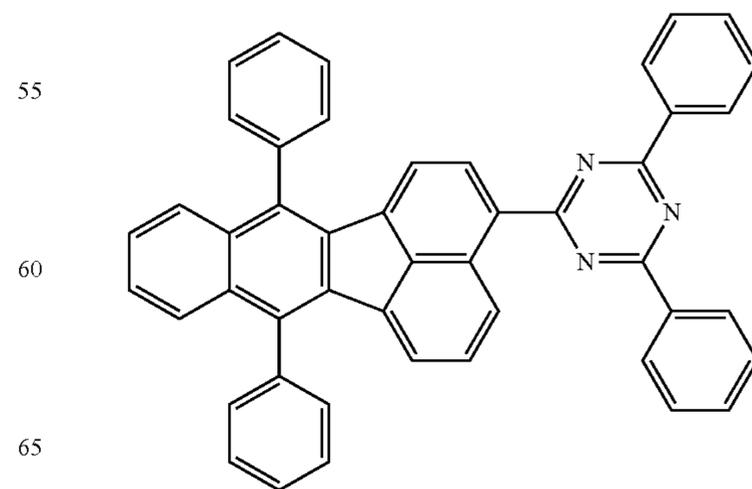
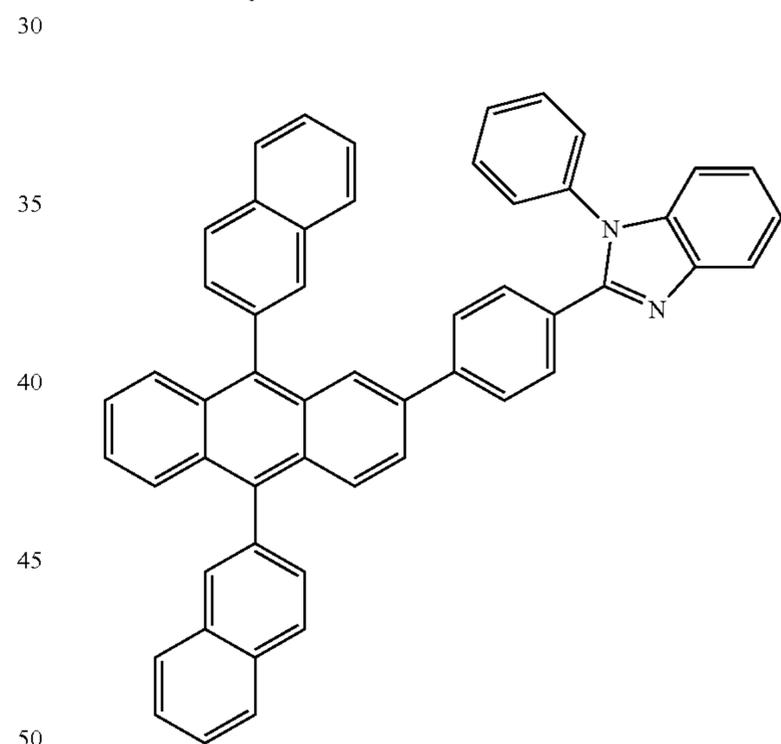
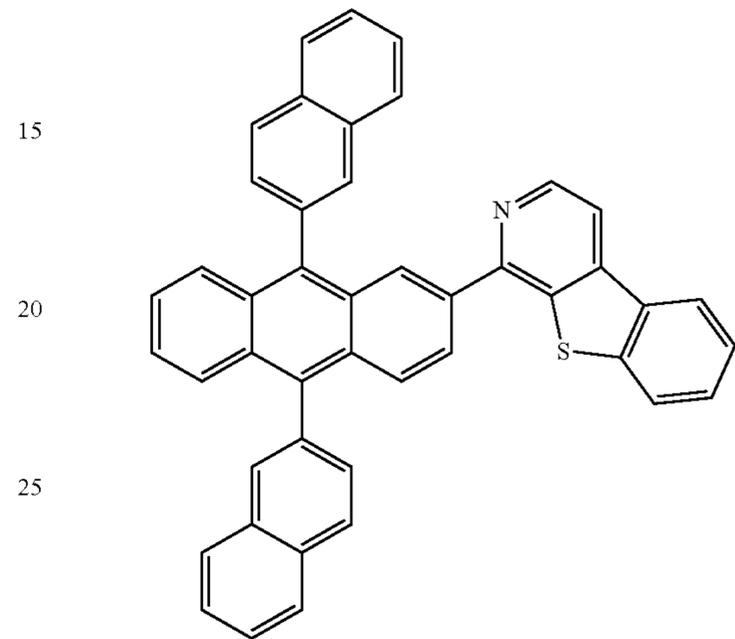
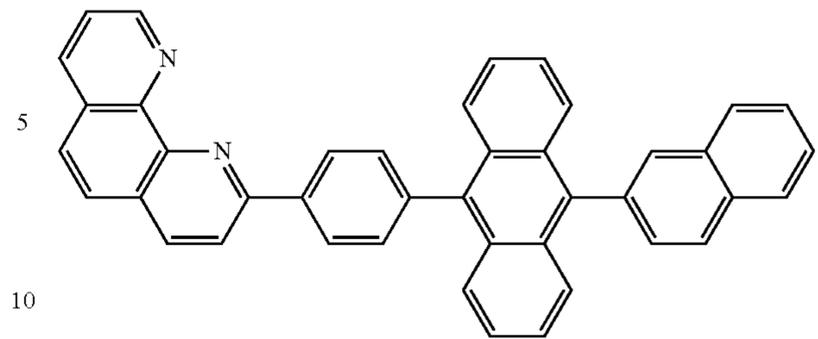
149

-continued



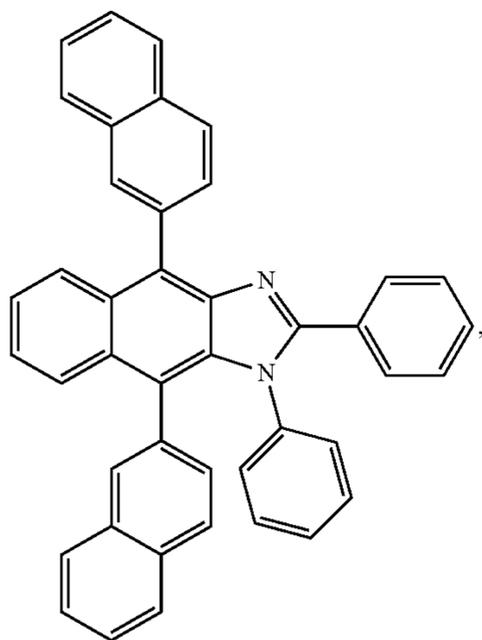
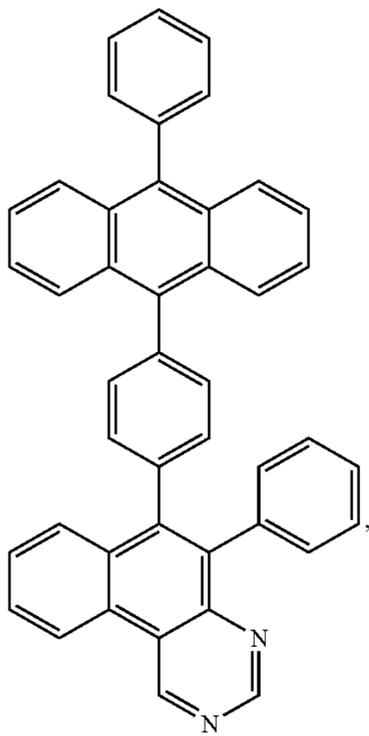
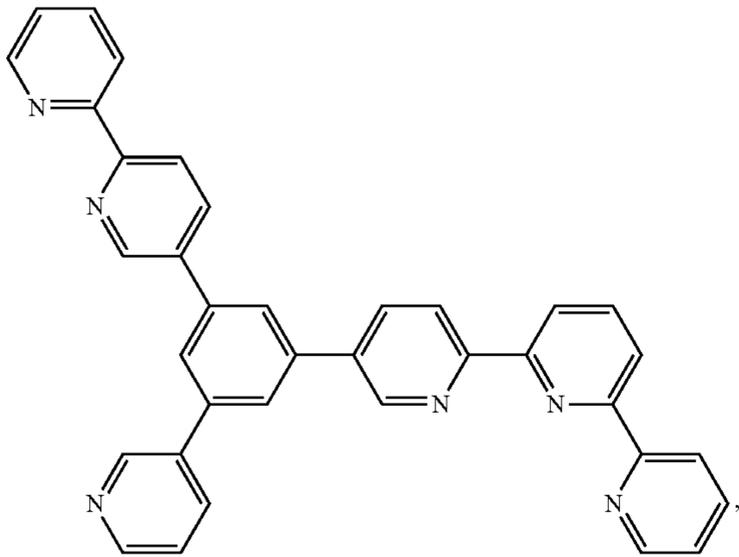
150

-continued



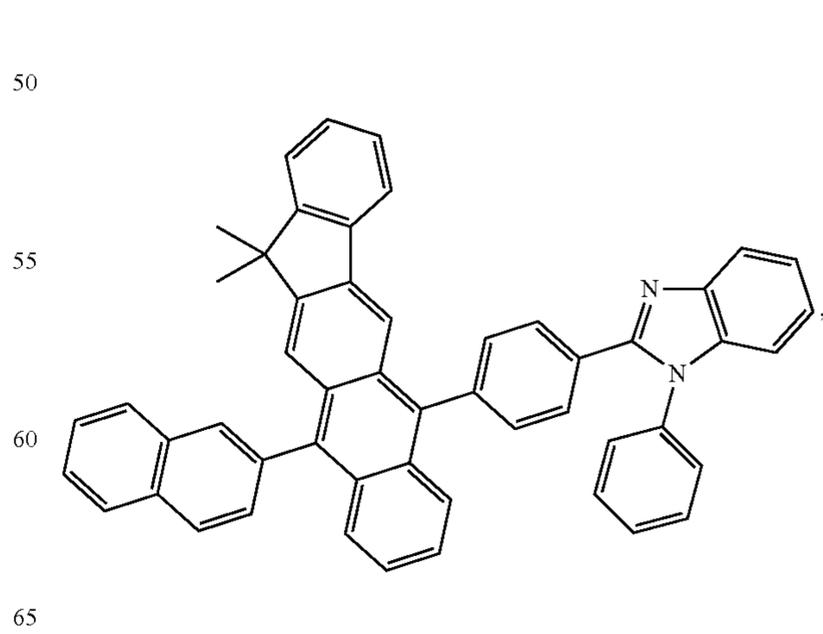
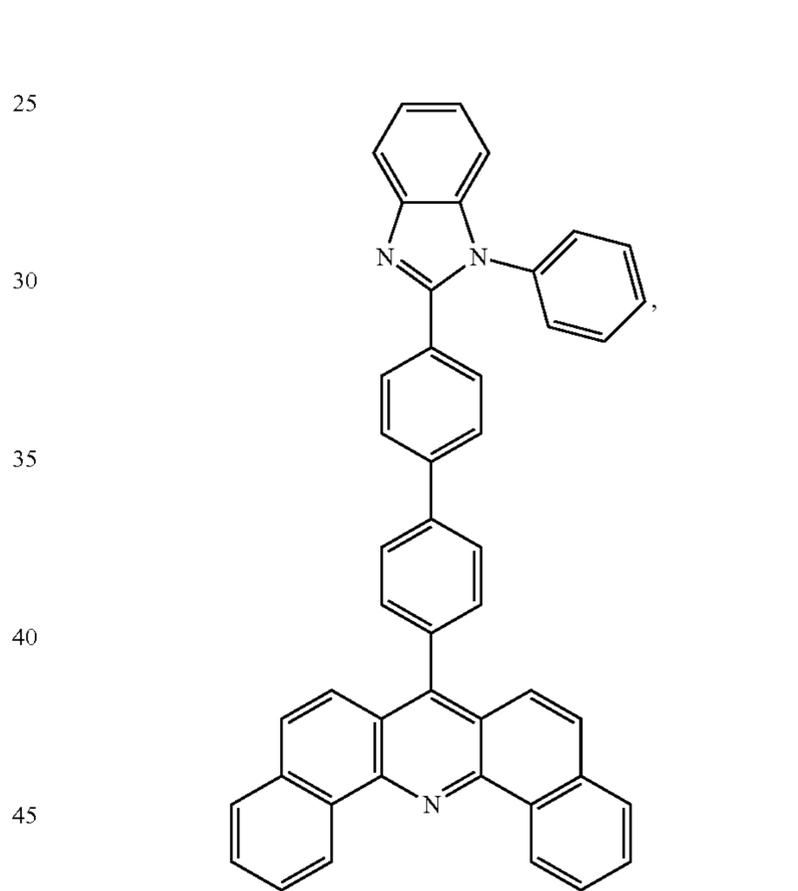
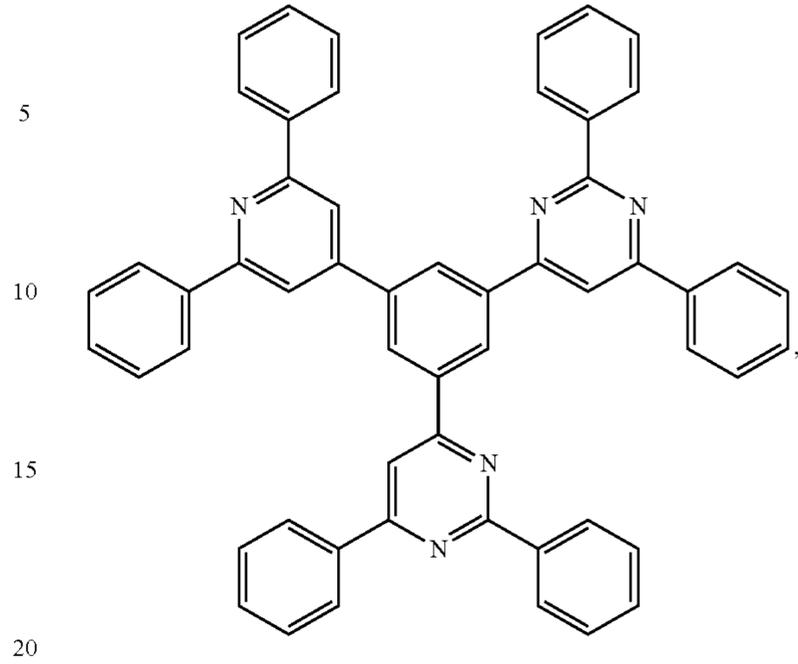
**151**

-continued



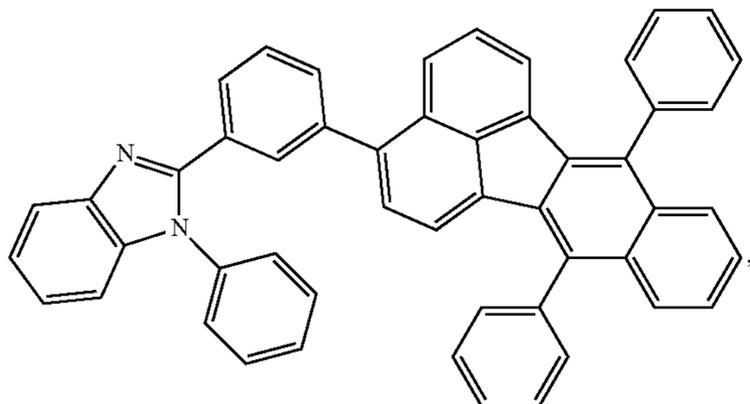
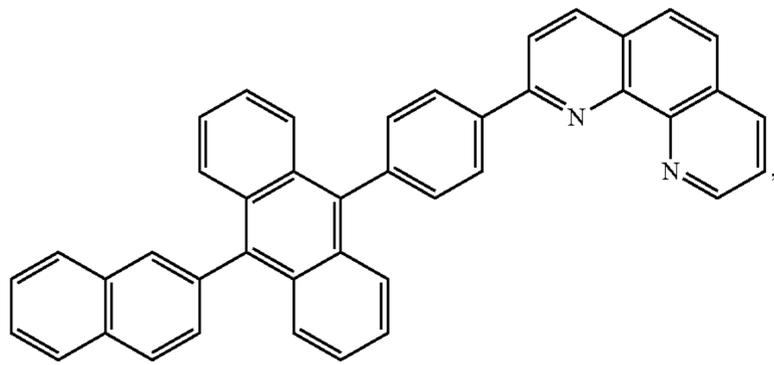
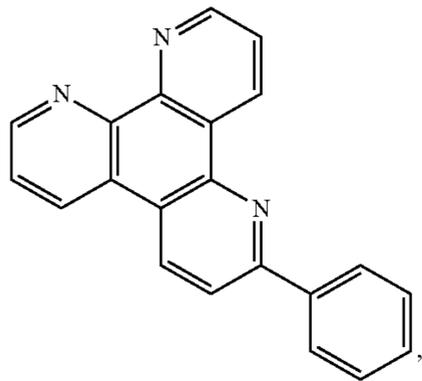
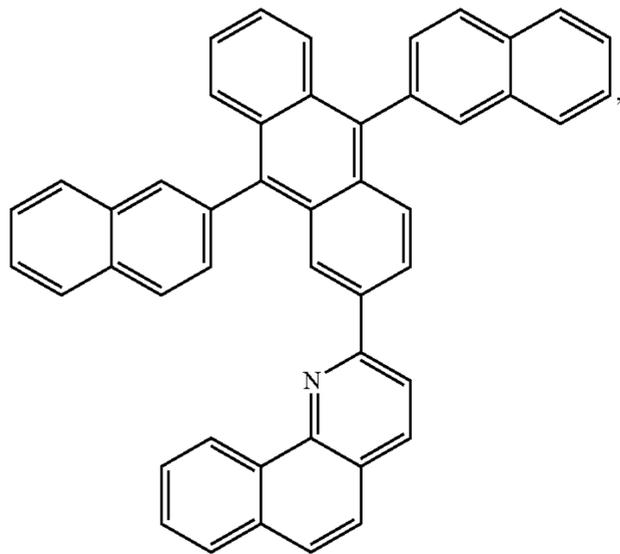
**152**

-continued



153

-continued



154

-continued

5

10

15

20

25

30

35

40

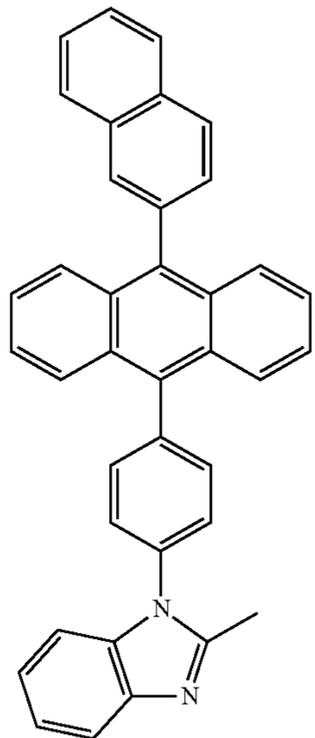
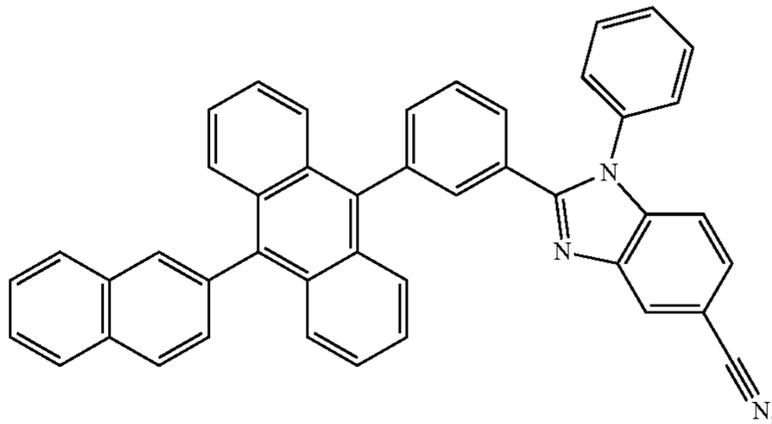
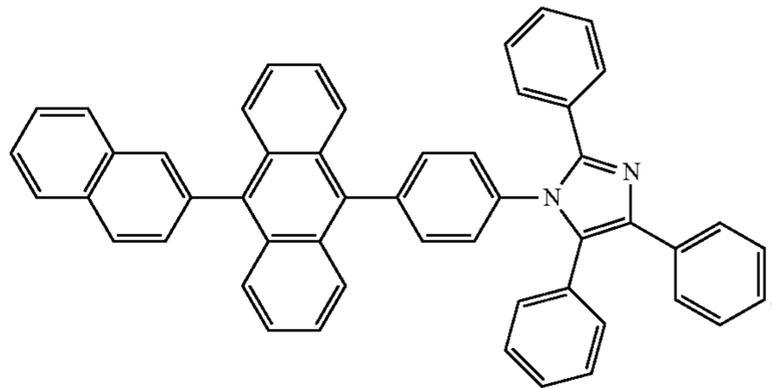
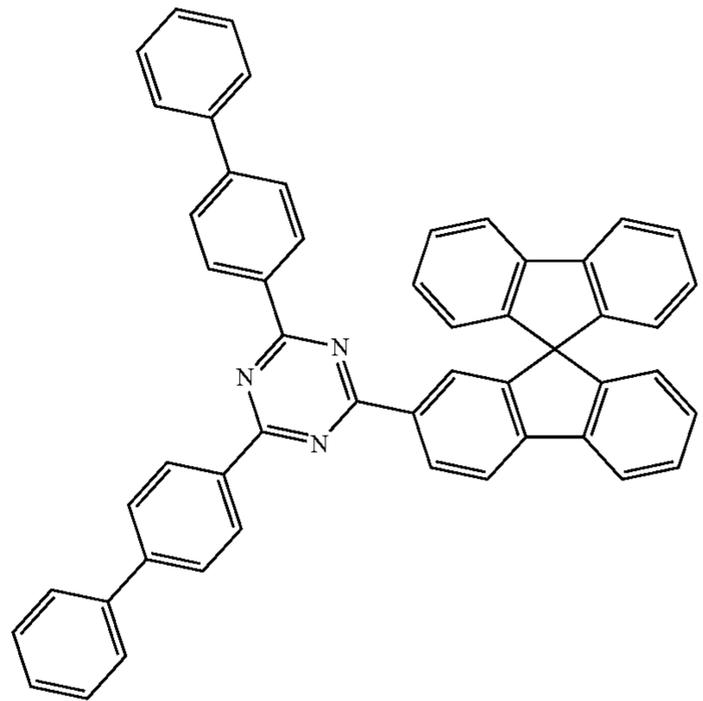
45

50

55

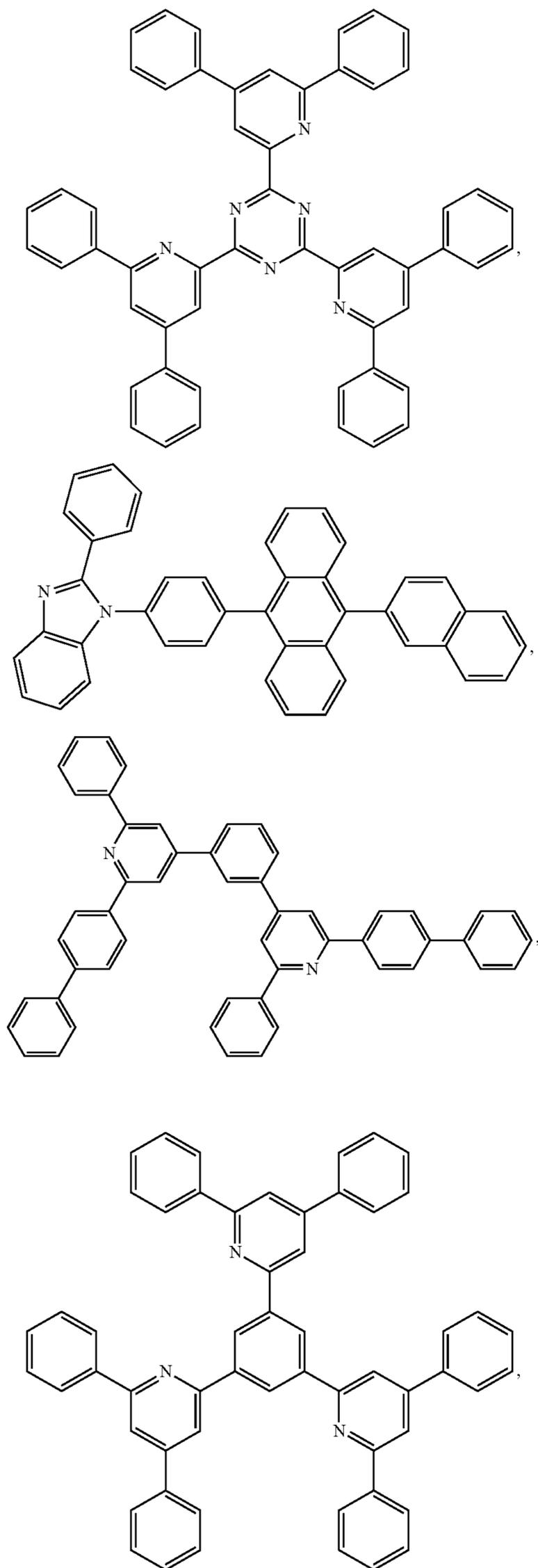
60

65



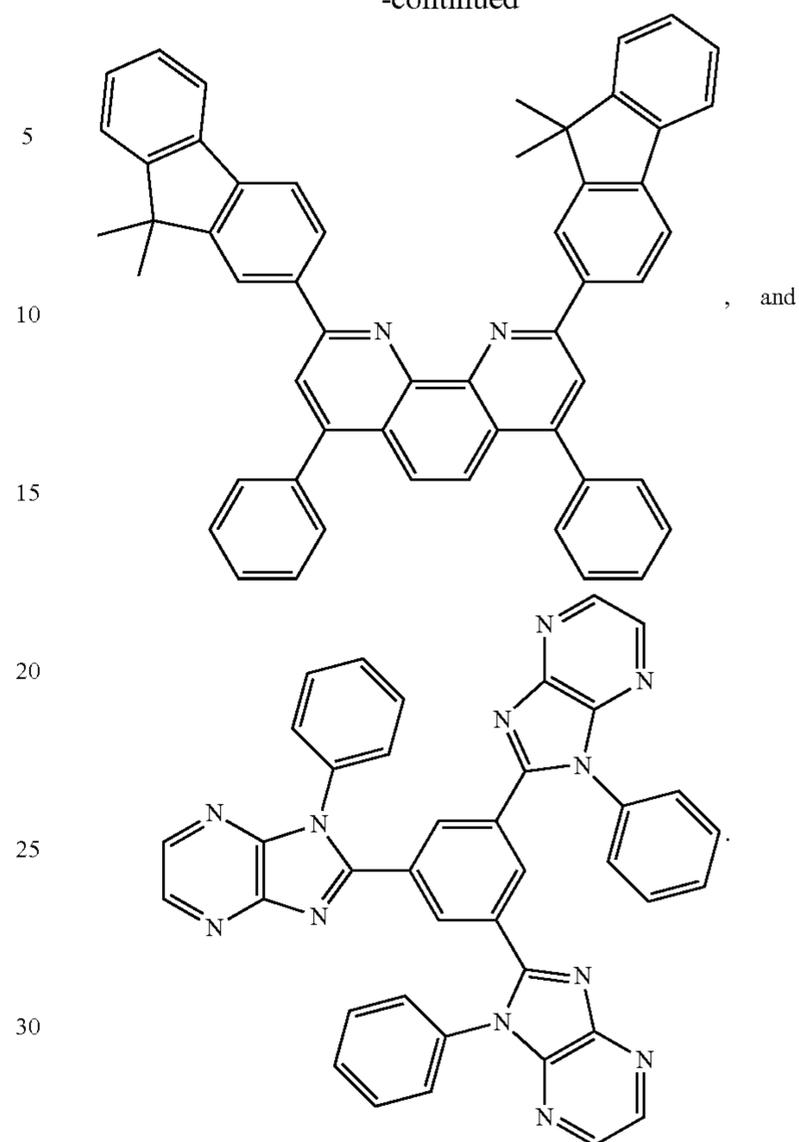
155

-continued



156

-continued



## 35 Charge Generation Layer (CGL)

In tandem or stacked OLEDs, the CGL plays an essential role in the performance, which is composed of an n-doped layer and a p-doped layer for injection of electrons and holes, respectively. Electrons and holes are supplied from the CGL and electrodes. The consumed electrons and holes in the CGL are refilled by the electrons and holes injected from the cathode and anode, respectively; then, the bipolar currents reach a steady state gradually. Typical CGL materials include n and p conductivity dopants used in the transport layers.

In any above-mentioned compounds used in each layer of the OLED device, the hydrogen atoms can be partially or fully deuterated. Thus, any specifically listed substituent, such as, without limitation, methyl, phenyl, pyridyl, etc. encompasses undeuterated, partially deuterated, and fully deuterated versions thereof. Similarly, classes of substituents such as, without limitation, alkyl, aryl, cycloalkyl, heteroaryl, etc. also encompass undeuterated, partially deuterated, and fully deuterated versions thereof.

## 55 EXPERIMENTAL

## Computational Examples

DFT calculations were carried out for the compounds shown below in TABLE 1 using the Gaussian software package (B3LYP/cep-31g) functional and basis set. TABLE 1 shows the calculated values for the HOMO and the LUMO, as well as singlet and triplet energy. The calculated triplet energy of Compounds 1, 5, 12, 23 and 139 are higher than the triplet energy of triphenylene, a well-studied compound for green PHOLED host construction. Although their triplet energy are lower than that of 1,3-Bis(N-carbazolyl) benzene (mCP), a commonly used host for blue PHOLED,

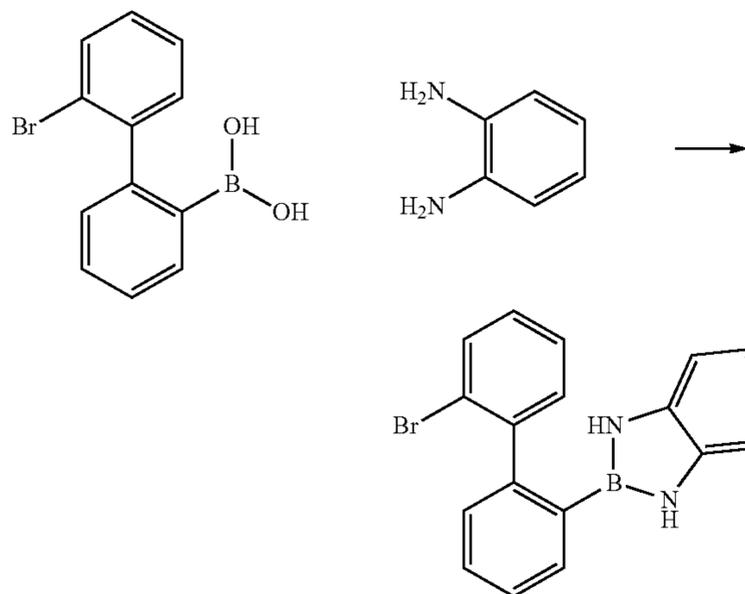
## 157

Compounds 1, 5, 12, 23 and 139 offer significantly more it delocalization as indicated by the lower HOMO-LUMO energy gap and lower LUMO due to their polyaromatic nature while maintaining relatively high triplet energy. Such features can improve OLED operation stability. The result indicates these boron nitrogen heterocycles are suitable as hosts for PHOLED.

Compound	HOMO (eV)	LUMO (eV)	T <sub>1</sub> (nm)
1	-5.59	-1.30	409
5	-5.49	-1.35	410
12	-5.71	-1.43	405
23	-5.72	-1.45	410
139	-5.62	-1.25	420
mCP	-5.41	-0.77	390
triphenylene	-5.85	-0.93	434

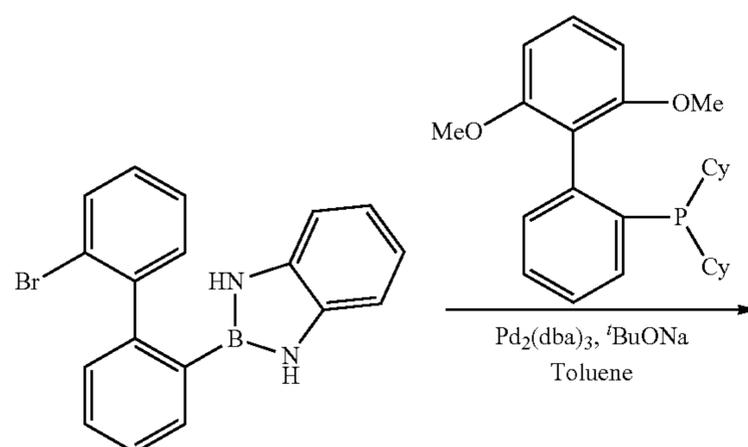
## Synthesis Examples

## Synthesis of 2-(2'-bromo-[1,1'-biphenyl]-2-yl)-2,3-dihydro-1H-benzo[d][1,3,2]diazaborole



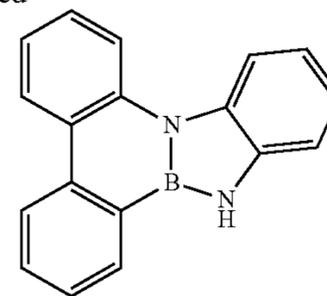
(2'-Bromo-[1,1'-biphenyl]-2-yl)boronic acid (2.77 g, 10 mmol) and 1,2-diaminobenzene (1.10 g, 10 mmol) were added to dry toluene (60 mL). The reaction mixture was refluxed for 2 hours, then water (2 mL) was removed by Dean-Stark distillation. The mixture was cooled to room temperature (~22° C.) and concentrated. The residue was purified by column chromatography using dichloromethane (DCM):hexane (1:4, v/v) as the eluent. 3.7 g (99%) of solid was obtained as the product, 2-(2'-bromo-[1,1'-biphenyl]-2-yl)-2,3-dihydro-1H-benzo[d][1,3,2]diazaborole.

## Synthesis of 10H-dibenzo[c,e]benzo[4,5][1,3,2]diazaborolo[1,2-a][1,2]azaborinine



## 158

-continued



5

10

15

20

25

30

35

40

45

50

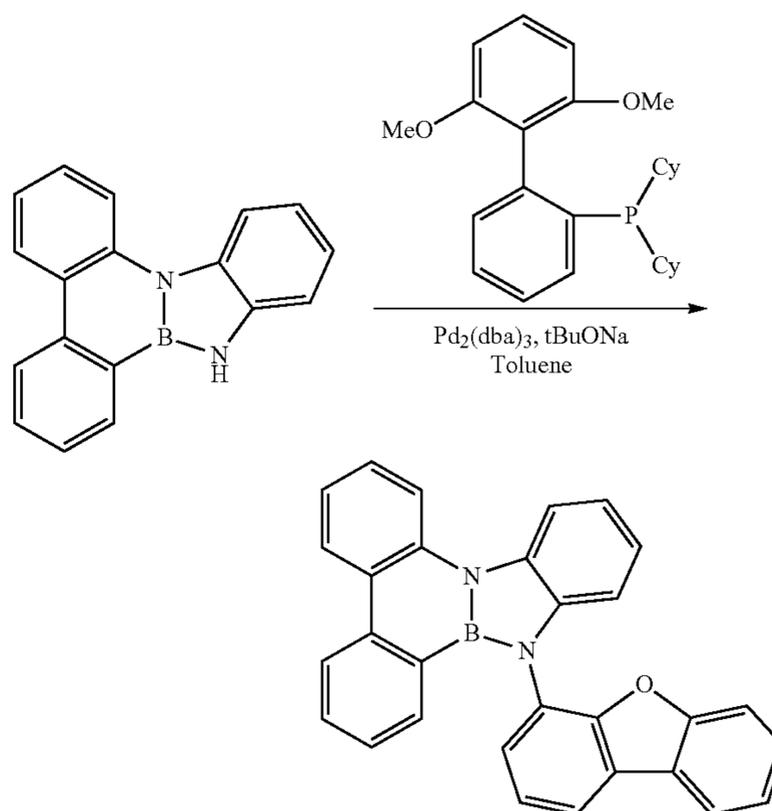
55

60

65

2-(2'-Bromo-[1,1'-biphenyl]-2-yl)-2,3-dihydro-1H-benzo[d][1,3,2]diazaborole (3.5 g, 10.0 mmol) was added to 250 mL of toluene. The solution was bubbled with nitrogen for 15 minutes, then tris(dibenzylideneacetone)dipalladium(0) [Pd<sub>2</sub>(dba)<sub>3</sub>] (0.1 g, 0.1 mmol), 2-dicyclohexylphosphino-2',6'-dimethoxybiphenyl (0.2 g, 0.5 mmol), and sodium tert-butoxide (1.5 g, 15 mmol) were added. The mixture was refluxed for 16 hours under nitrogen. After cooling to room temperature (~22° C.), the reaction mixture was filtered through silica gel and the filtrate was concentrated under reduced pressure. The residue was purified by column chromatography using DCM:hexane (1:4, v/v) as the eluent. 2.0 g (72%) of white solid was obtained as the product, 10H-dibenzo[c,e]benzo[4,5][1,3,2]diazaborolo[1,2-a][1,2]azaborinine.

## Synthesis of Compound 35

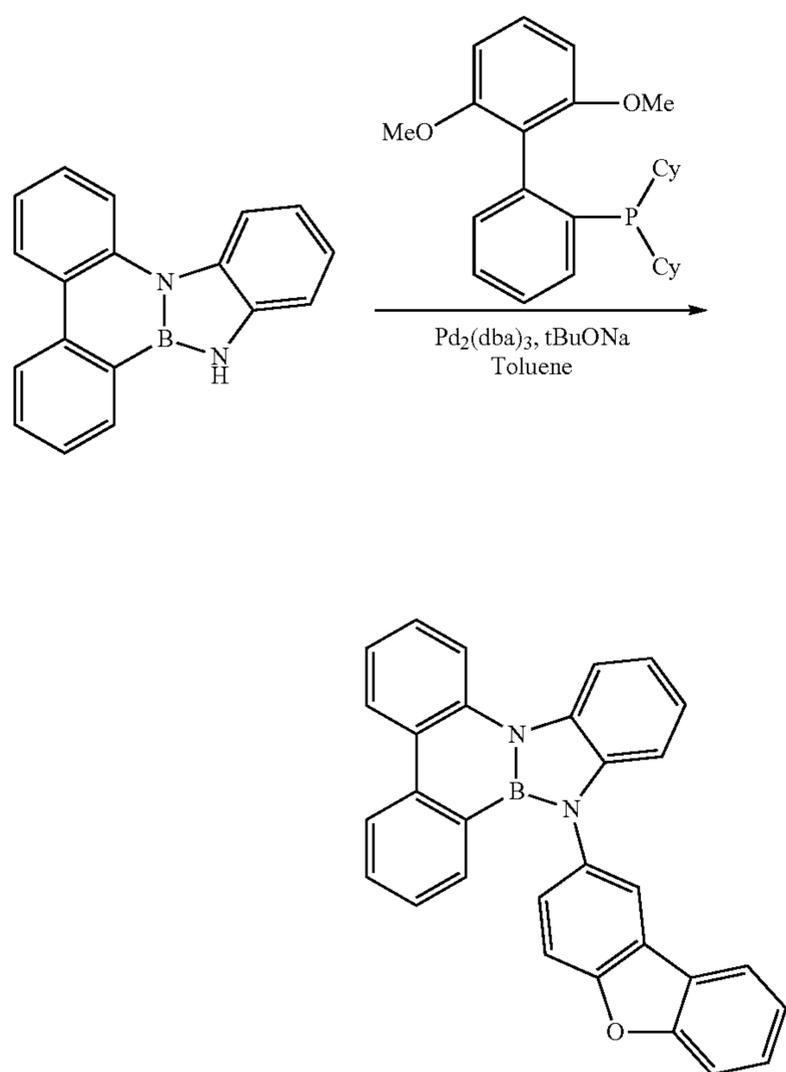


10H-dibenzo[c,e]benzo[4,5][1,3,2]diazaborolo[1,2-a][1,2]azaborinine (2.7 g, 10.0 mmol) and 4-bromodibenzofuran (3.0 g, 12.0 mmol) were added to 250 mL of toluene. The solution was bubbled with nitrogen for 15 min. Then Pd<sub>2</sub>(dba)<sub>3</sub> (0.1 g, 0.1 mmol), 2-dicyclohexylphosphino-2',6'-dimethoxybiphenyl (0.2 g, 0.5 mmol), and sodium tert-butoxide (1.5 g, 15 mmol) were added. The mixture was refluxed for 16 hours under nitrogen. After cooling to room temperature (~22° C.), the reaction mixture was filtered through silica gel and the filtrate was concentrated under reduced pressure. The residue was purified by column

159

chromatography using DCM:hexane (1:10, v/v) as the eluent. 3.5 g (79%) of white solid was obtained as Compound 35.

## Synthesis of Compound 37



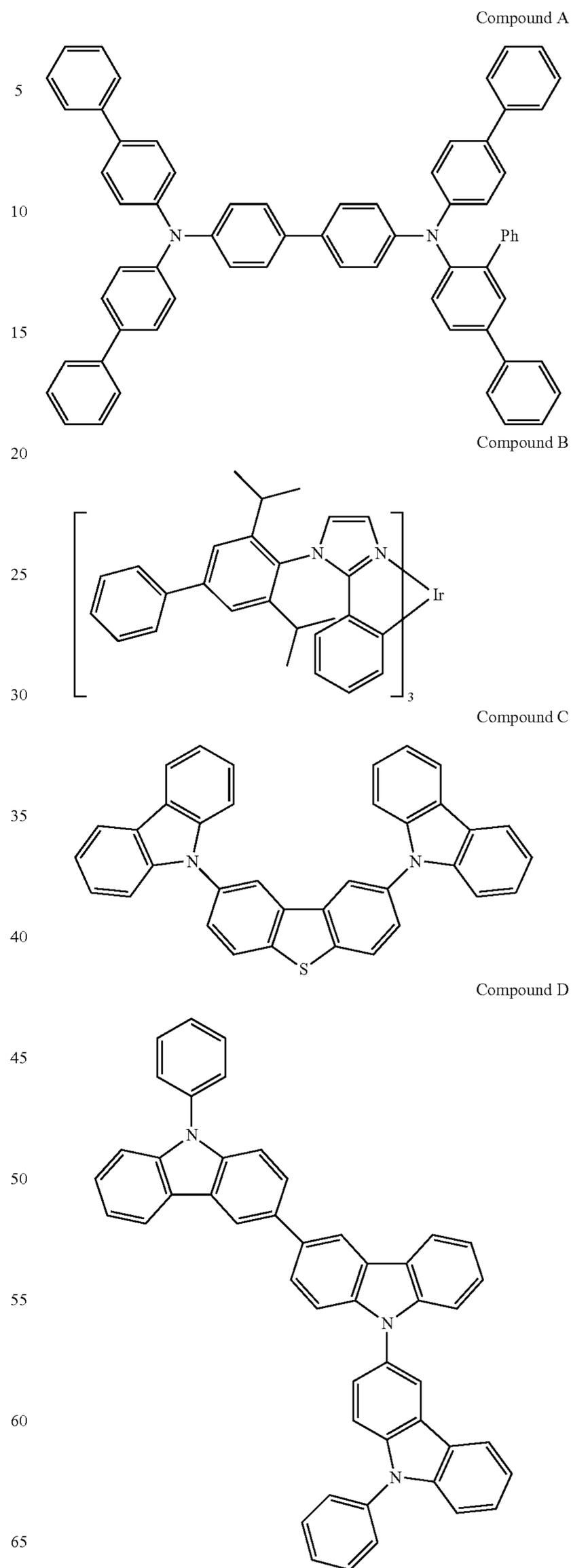
10H-dibenzo[c,e]benzo[4,5][1,3,2]diazaborolo[1,2-a][1,2]azaborinine (2.7 g, 10.0 mmol) and 2-bromodibenzofuran (3.0 g, 12.0 mmol) were added to 250 mL of toluene. The solution was bubbled with nitrogen for 15 min. Then,  $\text{Pd}_2(\text{dba})_3$  (0.1 g, 0.1 mmol), 2-dicyclohexylphosphino-2',6'-dimethoxybiphenyl (0.2 g, 0.5 mmol), and sodium tert-butoxide (1.5 g, 15 mmol) were added to the solution. The reaction mixture refluxed for 16 hours under nitrogen. After cooling to room temperature ( $\sim 22^\circ\text{C}$ ), the reaction mixture was filtered through silica gel and the filtrate was concentrated under reduced pressure. The residue was purified by column chromatography using DCM:hexane (1:10, v/v) as the eluent. 3.4 g (77%) of white solid was obtained as Compound 37.

## Device Examples

For the OLED experiment, all device examples were fabricated by high vacuum ( $<10^{-7}$  Torr) thermal evaporation. The anode electrode was  $\sim 800 \text{ \AA}$  of indium tin oxide (ITO). The cathode consisted of  $5 \text{ \AA}$  of LiF followed by  $1,000 \text{ \AA}$  of Al. All devices were encapsulated with a glass lid sealed with an epoxy resin in a nitrogen glove box ( $<1 \text{ ppm}$  of  $\text{H}_2\text{O}$  and  $\text{O}_2$ ) and a moisture getter was incorporated inside the package.

In addition to the compounds already disclosed herein, the following compounds were also used in the device examples.

160



## 161

## Device Example 1

The organic stack of the Device Examples in Table 1 consists of sequentially, from the ITO surface, 100 Å of LG101 (purchased from LG Chem. Korea) as the hole injection layer (HIL), 250 Å of Compound A as the hole transporting layer (HTL), 300 Å of Compound 35 doped with 20% of emitter Compound B as the emissive layer (EML), 50 Å of Compound C as electron transport layer 2 (ETL2), and 300 Å of Alq<sub>3</sub> as electron transport layer 1 (ETL1).

Device Example 2 and Device Comparative Example 1 were fabricated in the same way except the host materials were Compound 37 and Compound C, respectively.

## Device Example 3

The organic stack of the Device Examples in Table 1 consists of sequentially, from the ITO surface, 100 Å of LG101 (purchased from LG Chem. Korea) as the hole injection layer (HIL), 250 Å of Compound A as the hole transporting layer (HTL), 50 Å of Compound D as the blocking layer (BL), 300 Å of Compound 35 doped with 20% of emitter Compound B as the emissive layer (EML), 50 Å of Compound C as ETL2, and 300 Å of Alq<sub>3</sub> as ETL1.

Device Example 4 and Device Comparative Example 2 were fabricated in the same way except the host materials were Compound 37 and Compound C, respectively.

The device data is summarized in Table 2, below.

Device	Host	At 1,000 cd/m <sup>2</sup>						
		1931 CIE		Em <sub>max</sub>	Voltage	LE	EQE	PE
		x	y	[nm]	[V]	[cd/A]	[%]	[lm/W]
Example 1	Cmpd 35	0.172	0.386	474	5.2	46.9	21.2	28.2
Example 2	Cmpd 37	0.173	0.378	474	5.3	44.1	20.2	26.3
Comparative Example 1	Cmpd C	0.171	0.383	474	5.2	45.8	20.9	27.5
Example 3	Cmpd 35	0.174	0.395	474	5.2	59.2	26.3	36.1
Example 4	Cmpd 37	0.173	0.385	474	5.2	54.1	24.5	32.8
Comparative Example 2	Cmpd C	0.173	0.393	474	5.2	54.8	24.5	32.8

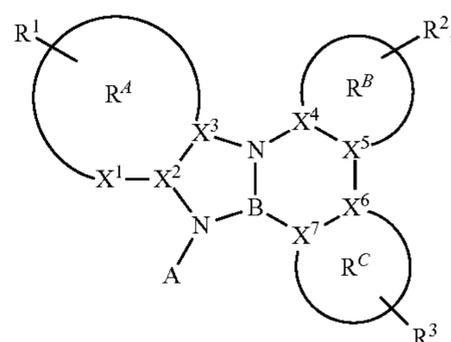
The results in Table 2 indicate that the Compounds of Formula I have similar or better performance for OLED application, especially as hosts, when they are compared with the state of the art blue host, Compound C.

It is understood that the various embodiments described herein are by way of example only, and are not intended to limit the scope of the invention. For example, many of the materials and structures described herein may be substituted with other materials and structures without deviating from the spirit of the invention. The present invention as claimed may therefore include variations from the particular examples and preferred embodiments described herein, as will be apparent to one of skill in the art. It is understood that various theories as to why the invention works are not intended to be limiting.

## 162

We claim:

1. A compound having a structure of Formula I:



Formula I

wherein R<sup>A</sup>, R<sup>B</sup>, and R<sup>C</sup> are each independently 5 or 6 membered aryl or heteroaryl rings;

wherein R<sup>1</sup>, R<sup>2</sup>, and R<sup>3</sup> each independently represent no substitutions or up to the maximum available substitutions;

wherein R<sup>1</sup>, R<sup>2</sup>, and R<sup>3</sup> are each independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphine, a substituent of Formula I, and combinations thereof;

wherein any adjacent R<sup>1</sup>, R<sup>2</sup>, and R<sup>3</sup> are optionally joined or fused to form a ring;

wherein A is selected from the group consisting of halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, ary-

loxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphine, a substituent of Formula I, partially or fully deuterated variants thereof, and combinations thereof;

wherein A is optionally bonded to at least one benzo or azabenzene ring to form fused rings;

wherein X<sup>1</sup> is B, C, N, O, S or Se; and

wherein X<sup>2</sup>-X<sup>7</sup> are independently B, C or N.

2. The compound of claim 1, wherein A is aryl or heteroaryl.

3. The compound of claim 1, wherein A is selected from the group consisting of phenyl, carbazole, azacarbazole, dibenzofuran, dibenzothiophene, dibenzoselenophene, azadibenzofuran, azadibenzothiophene, azadibenzoselenophene, triphenylene, azatriphenylene, and combinations thereof;

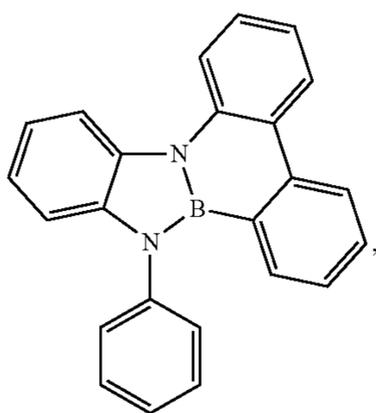
163

wherein A is optionally further substituted by one or more substituent B;

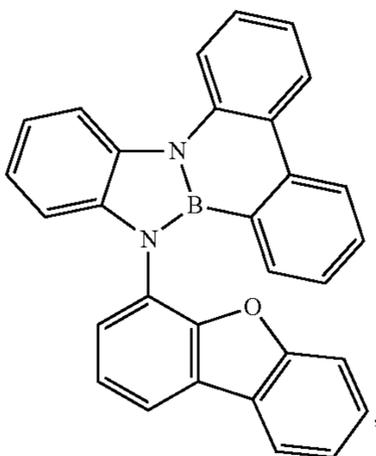
wherein B is selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphine, and combinations thereof; and

wherein B is optionally bonded to at least one benzo or azabenz ring to form a fused ring.

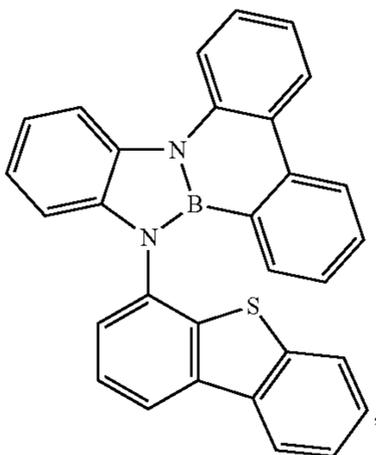
4. The compound of claim 3, wherein the compound is selected from the group consisting of:



Compound 34



Compound 35

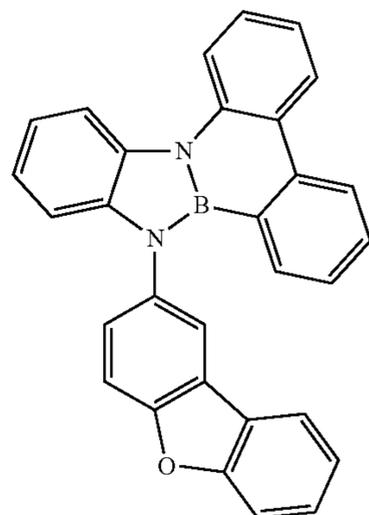


Compound 36

164

-continued

Compound 37



5

10

15

20

25

30

35

40

45

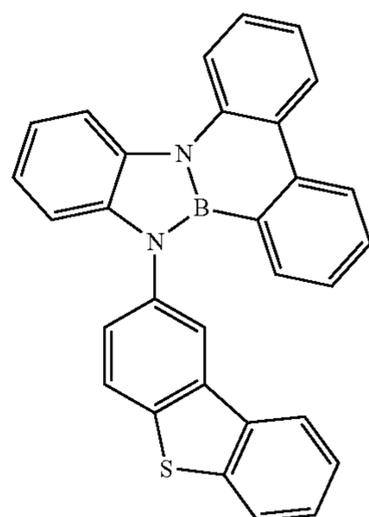
50

55

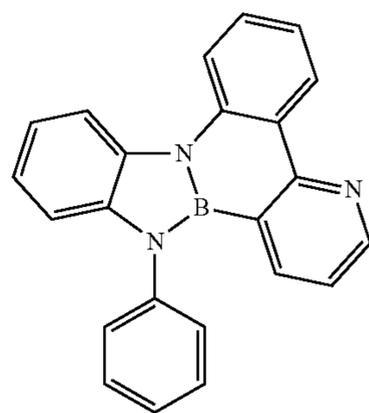
60

65

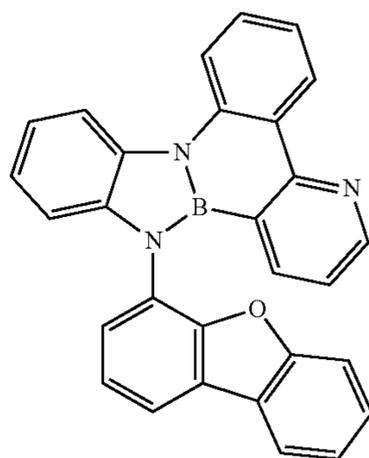
Compound 38



Compound 39

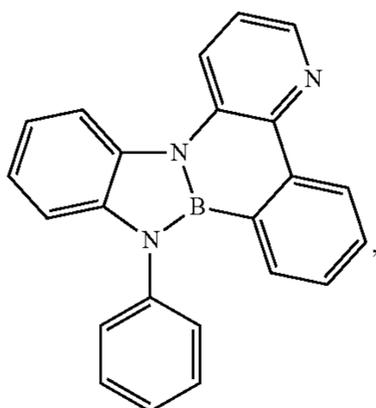
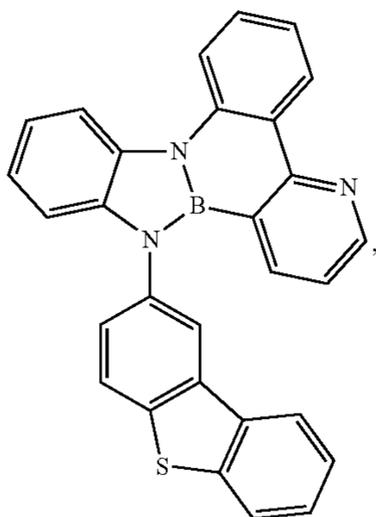
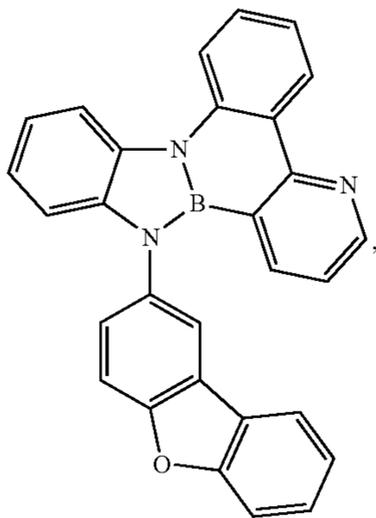
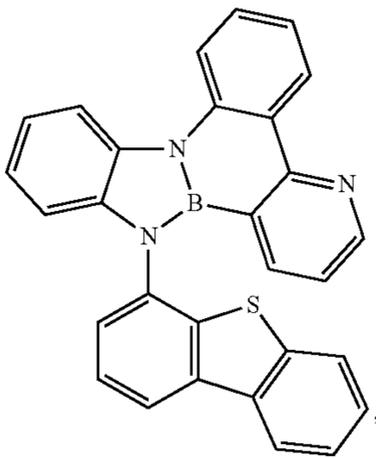


Compound 40



**165**

-continued



**166**

-continued

Compound 41

5

10

15

Compound 42

20

25

30

Compound 43

35

40

45

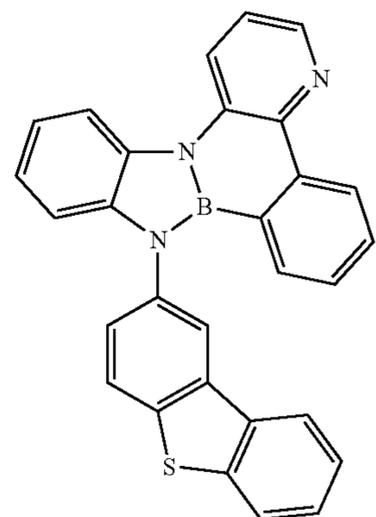
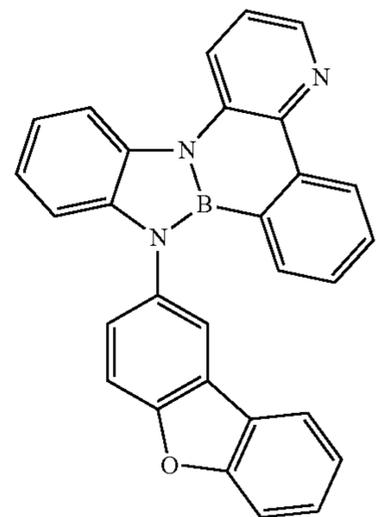
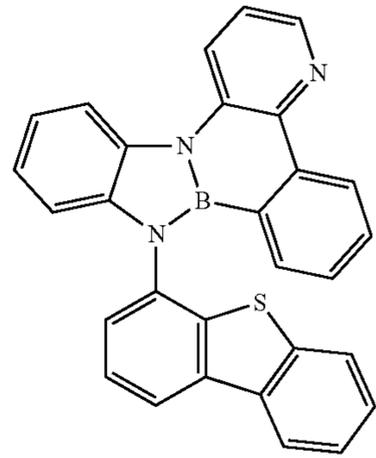
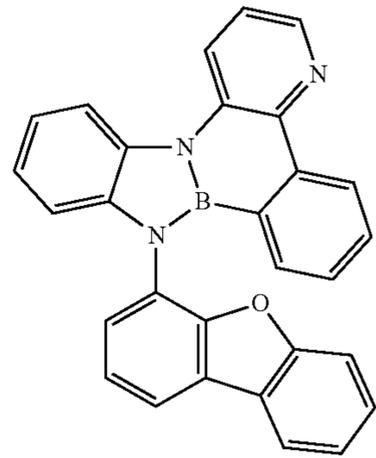
50

Compound 44

55

60

65



Compound 45

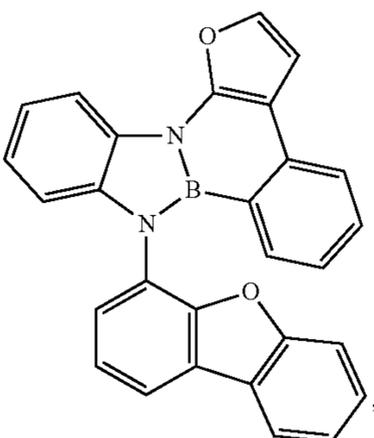
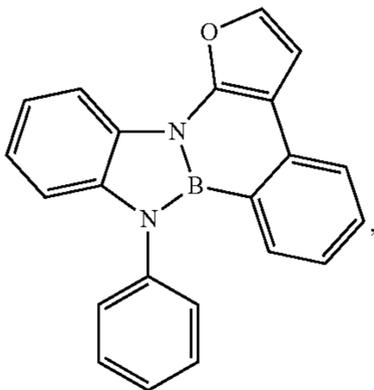
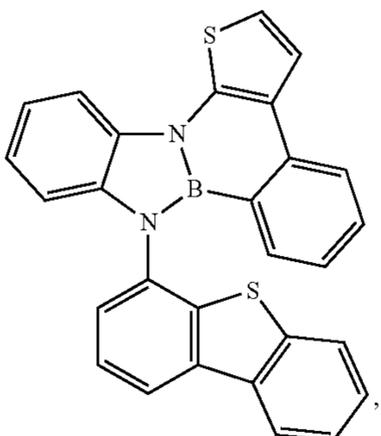
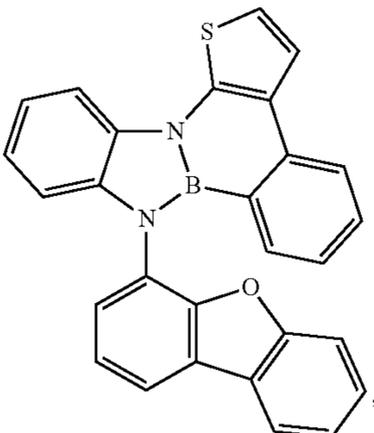
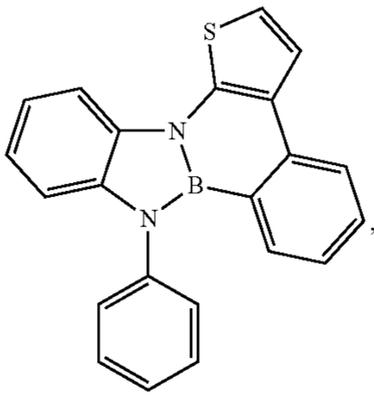
Compound 46

Compound 47

Compound 48

**167**

-continued

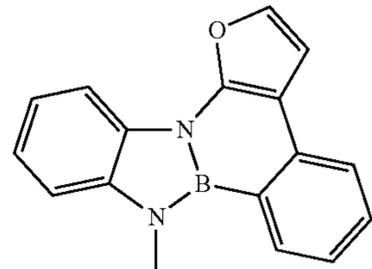


**168**

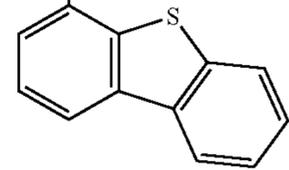
-continued

Compound 79

5

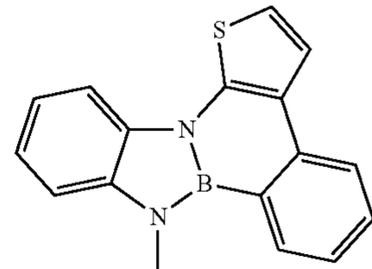


10



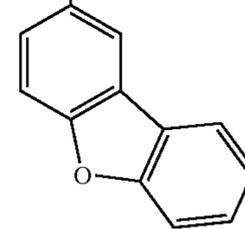
Compound 80

15



20

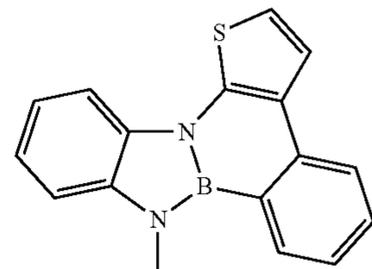
25



Compound 81

30

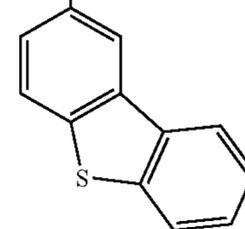
35



40

Compound 82

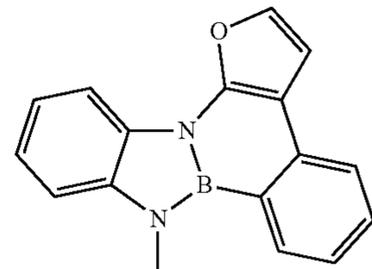
45



50

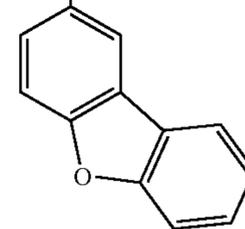
Compound 83

55



60

65



Compound 84

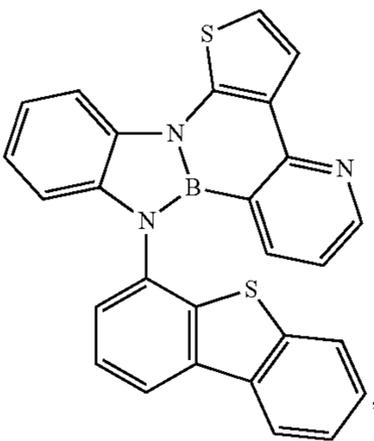
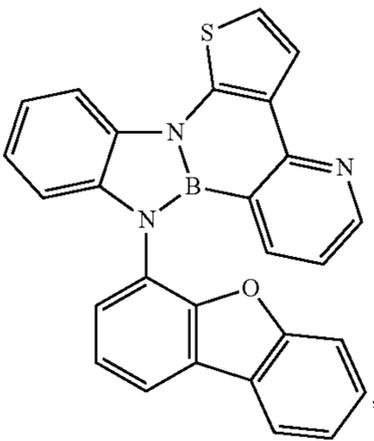
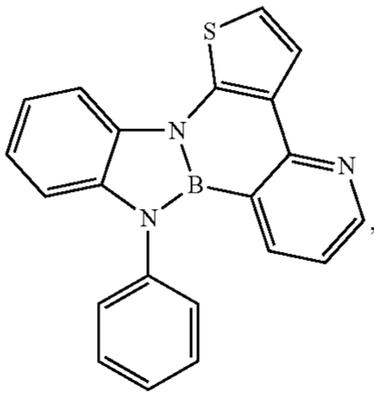
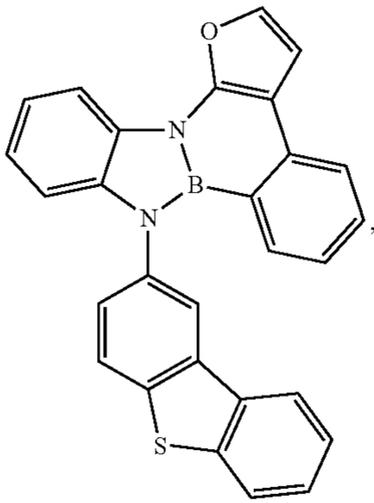
Compound 85

Compound 86

Compound 87

**169**

-continued

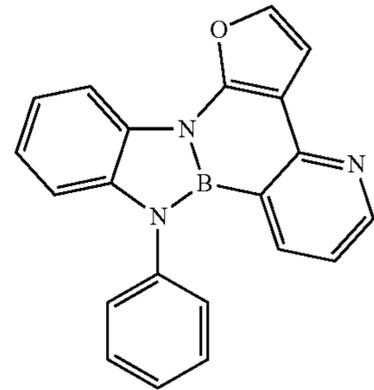


**170**

-continued

Compound 88

5



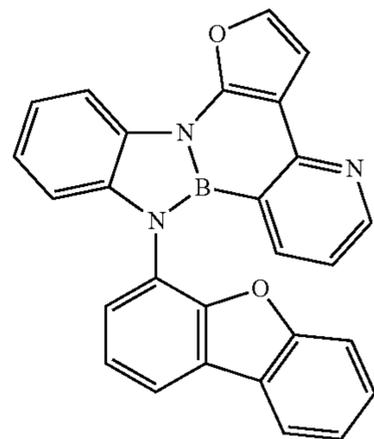
10

15

Compound 89

20

25



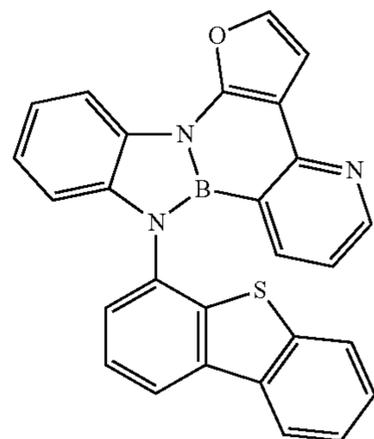
30

Compound 90

35

40

45



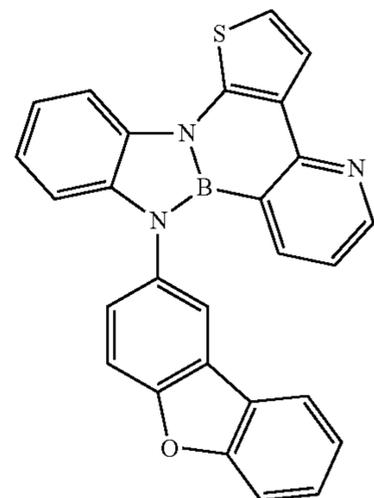
50

Compound 91

55

60

65



Compound 92

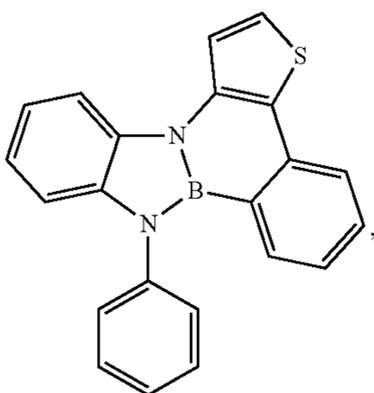
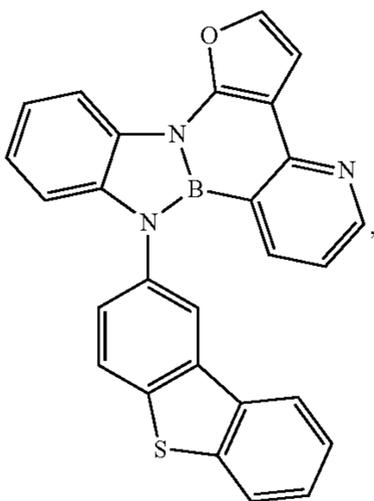
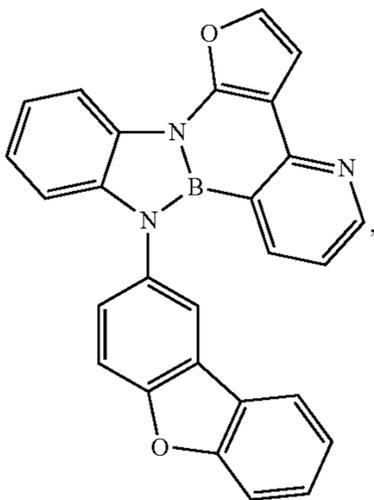
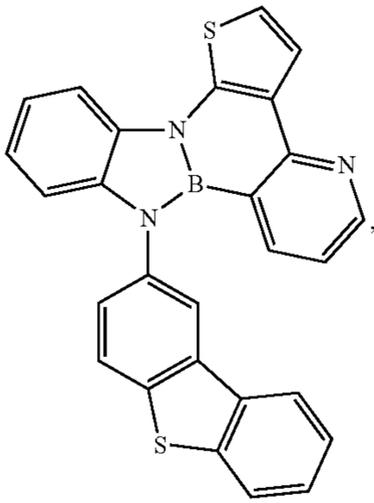
Compound 93

Compound 94

Compound 95

**171**

-continued

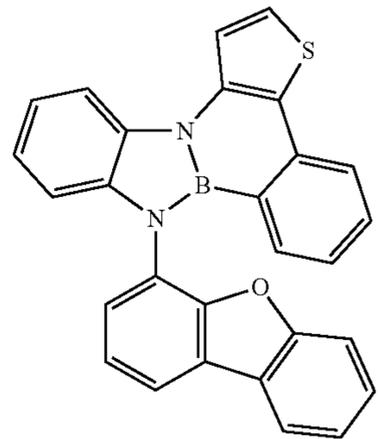


**172**

-continued

Compound 96

5

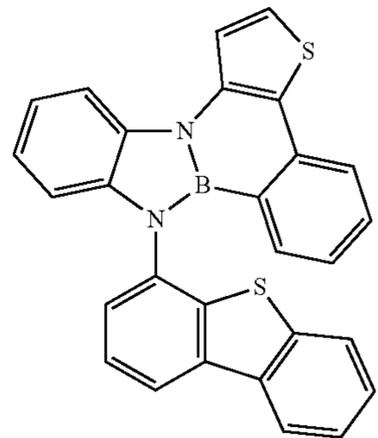


10

15

Compound 97

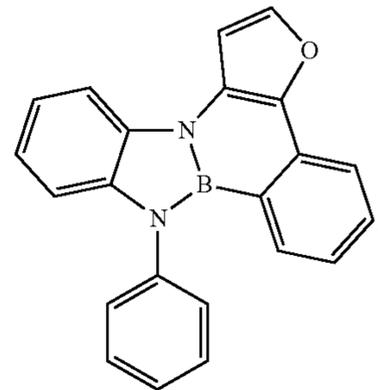
20



25

Compound 98

40

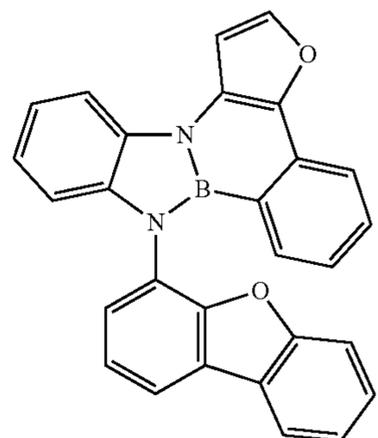


30

35

Compound 99

55



45

50

65

Compound 100

Compound 101

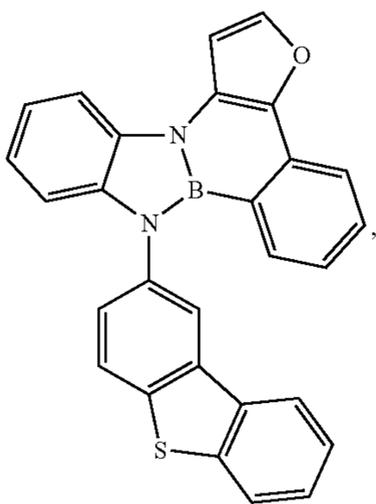
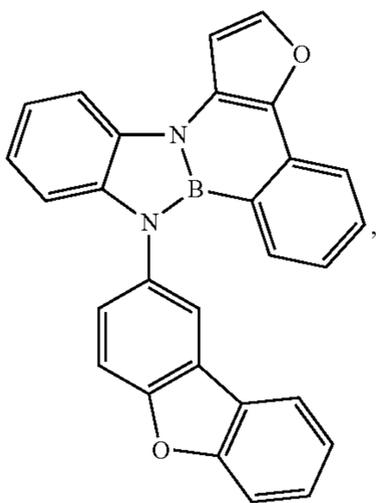
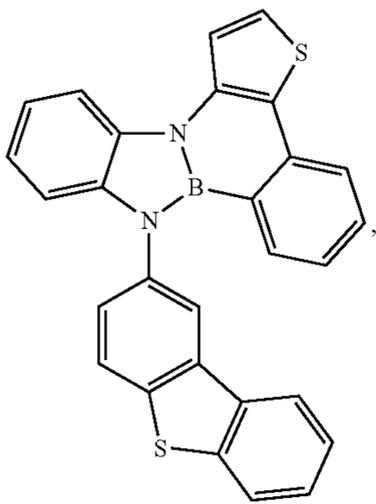
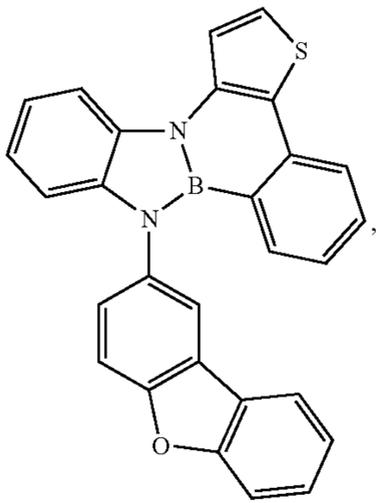
Compound 102

Compound 103

Compound 104

**173**

-continued

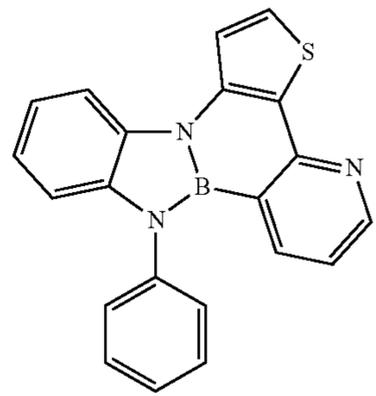


**174**

-continued

Compound 105

5



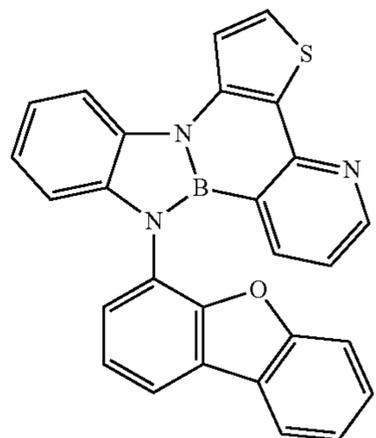
Compound 109

10

15

Compound 106

20



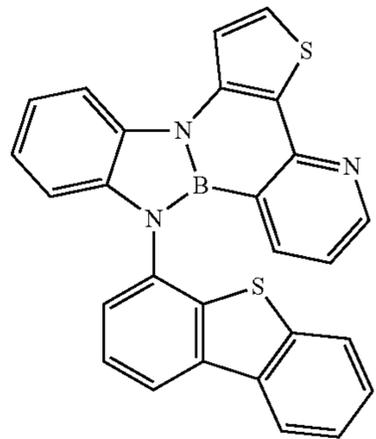
Compound 110

25

30

Compound 107

35



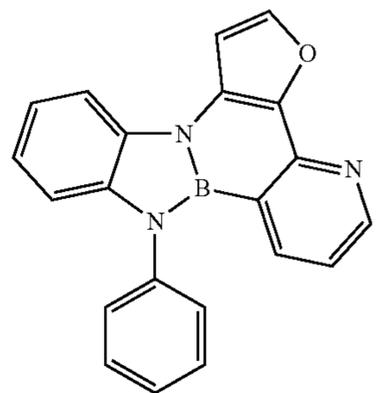
Compound 111

40

45

Compound 108

50

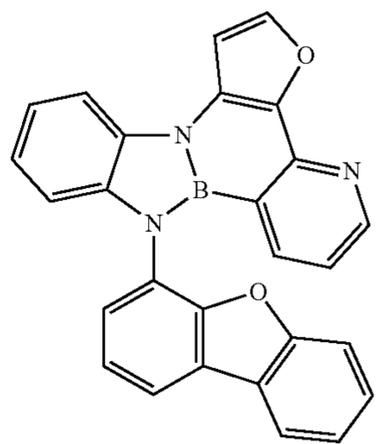


Compound 112

55

60

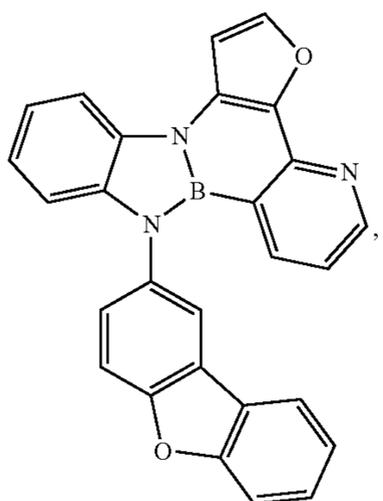
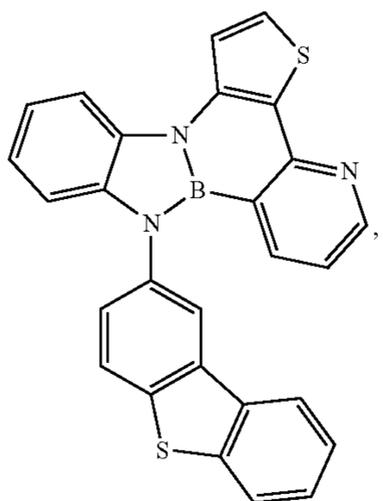
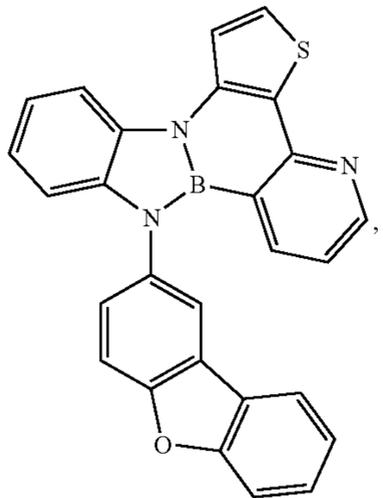
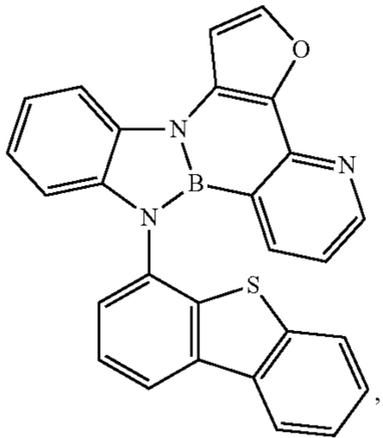
65



Compound 113

**175**

-continued

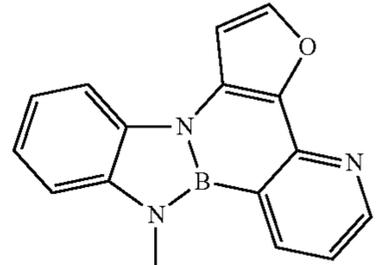


**176**

-continued

Compound 114

5

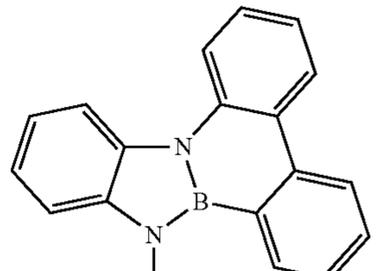


10

15

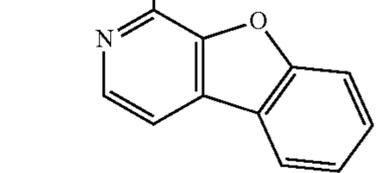
Compound 115

20



25

30



Compound 116

35

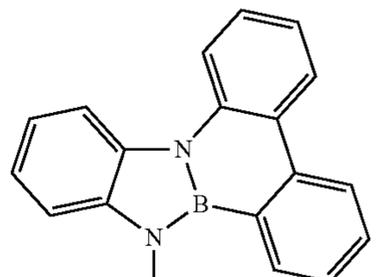
Compound 118

Compound 119

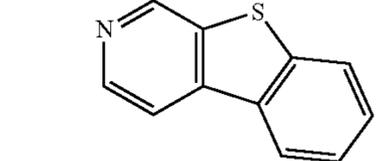
Compound 120

Compound 117

40



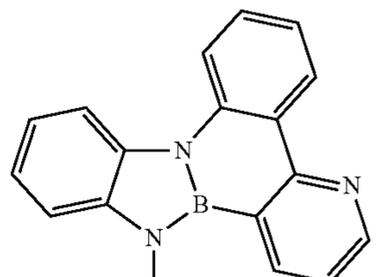
45



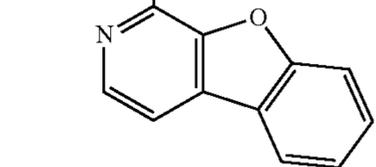
50

Compound 117

55



60

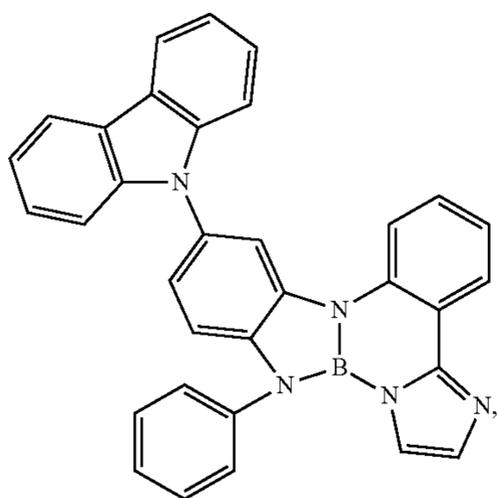
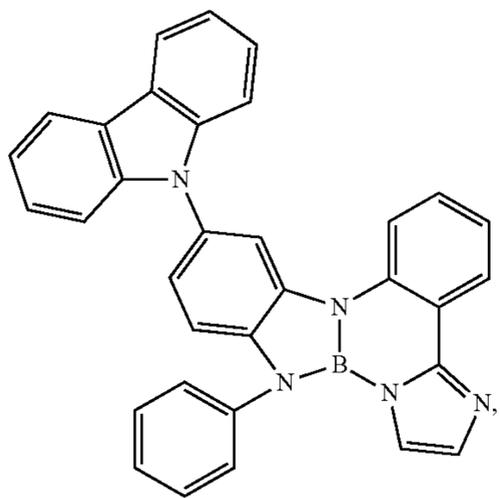
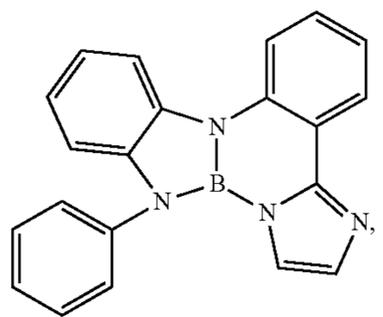
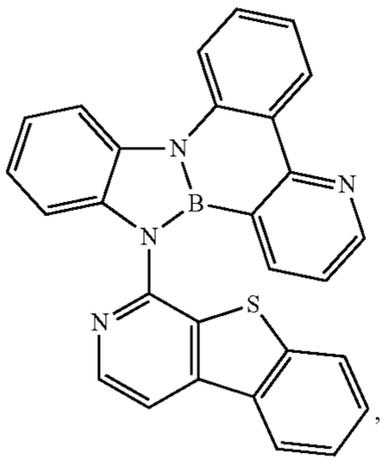


65

Compound 121

177

-continued



178

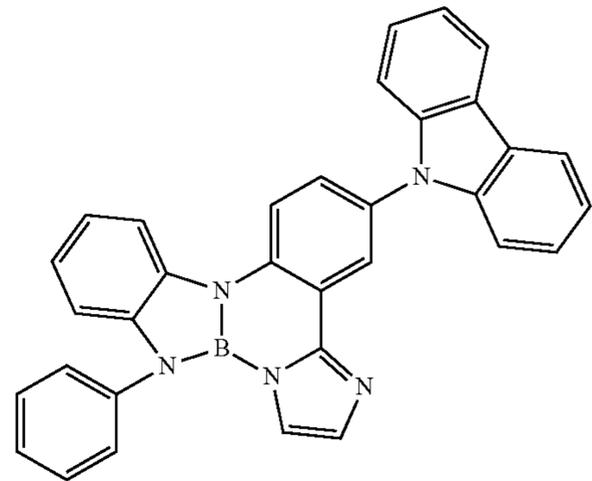
-continued

Compound 122

5

10

15



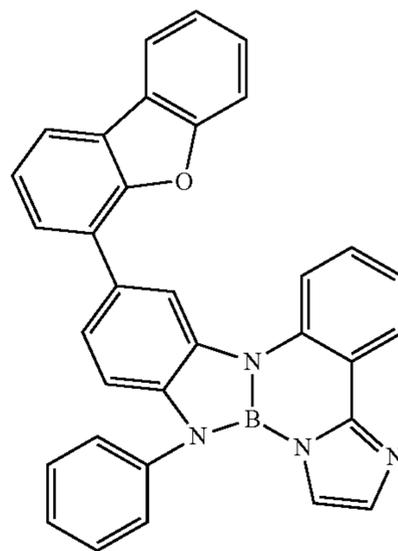
Compound 126

Compound 123

20

25

30



Compound 127

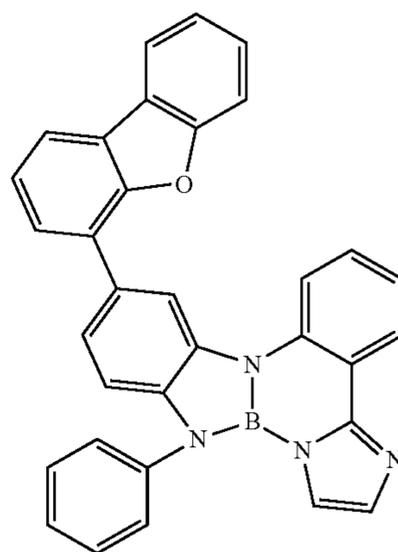
Compound 124

35

40

45

50



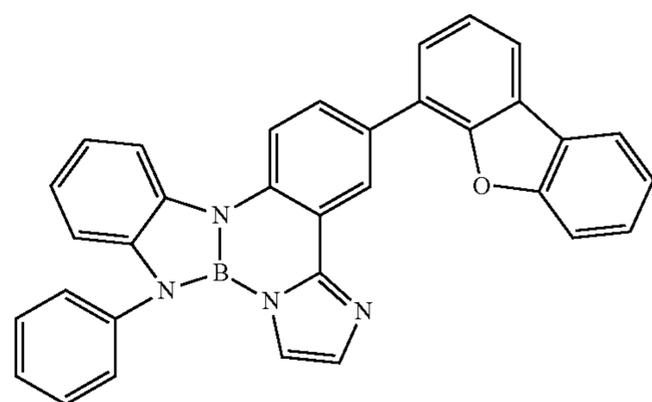
Compound 128

Compound 125

55

60

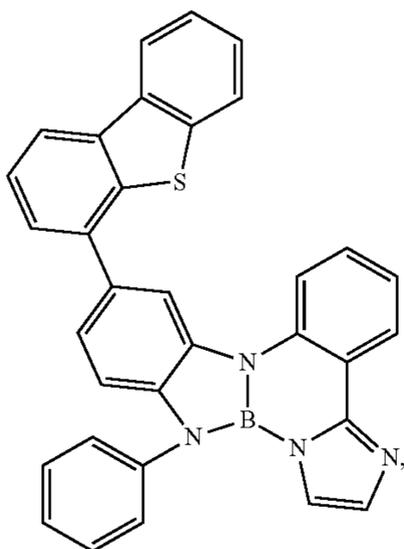
65



Compound 129

179

-continued



Compound 130

5

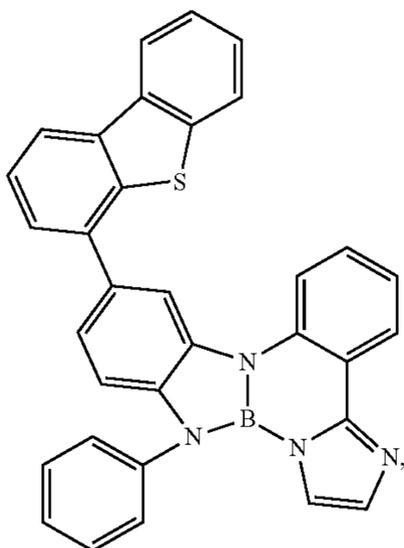
10

15

Compound 131

20

25

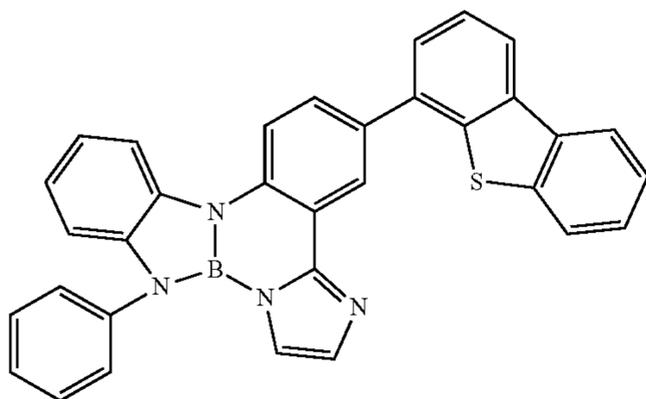


Compound 132

35

40

45



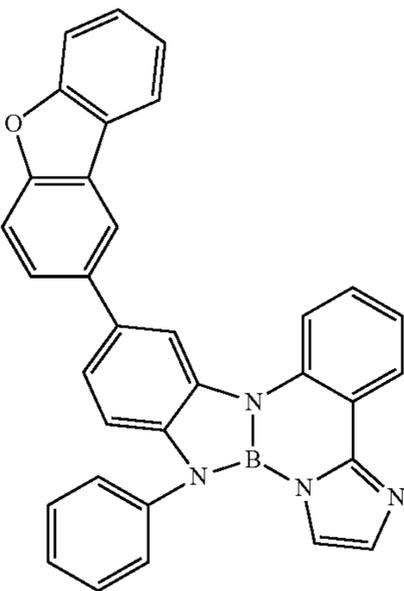
Compound 133

50

55

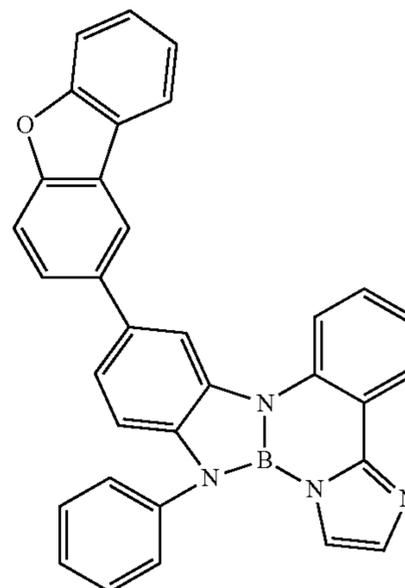
60

65

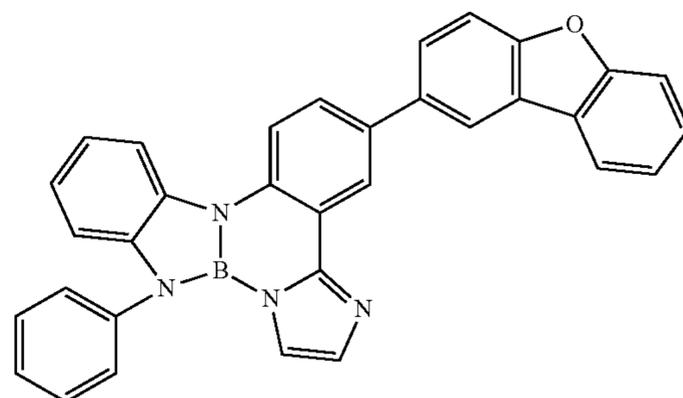


180

-continued

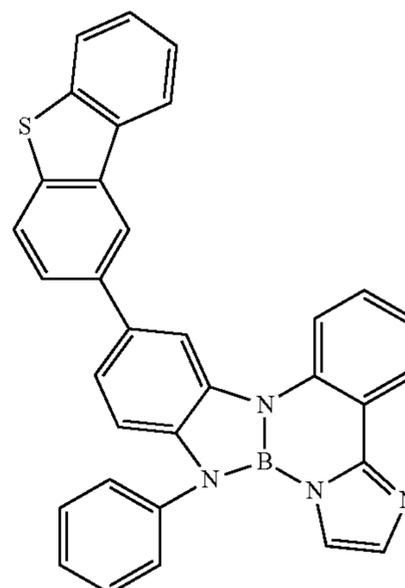


Compound 134



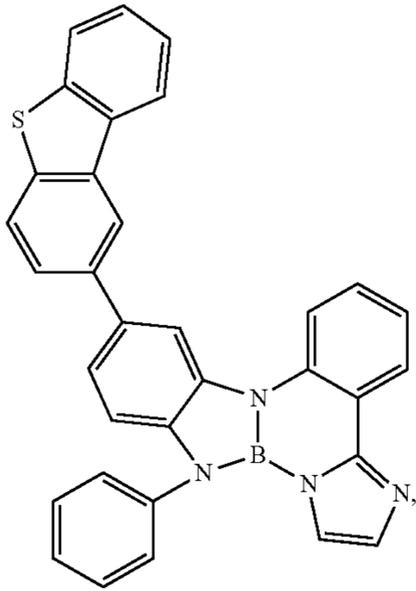
Compound 135

Compound 136

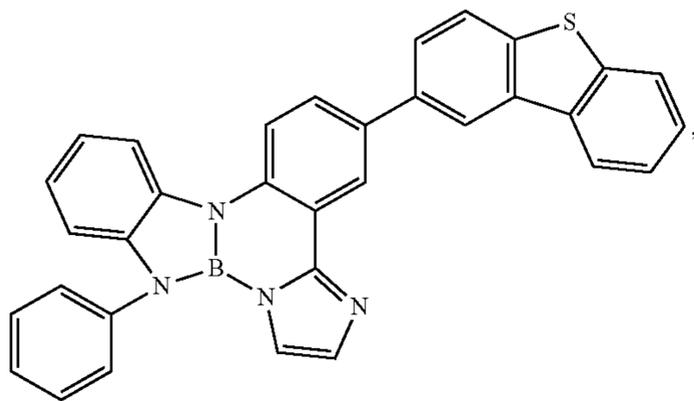


**181**

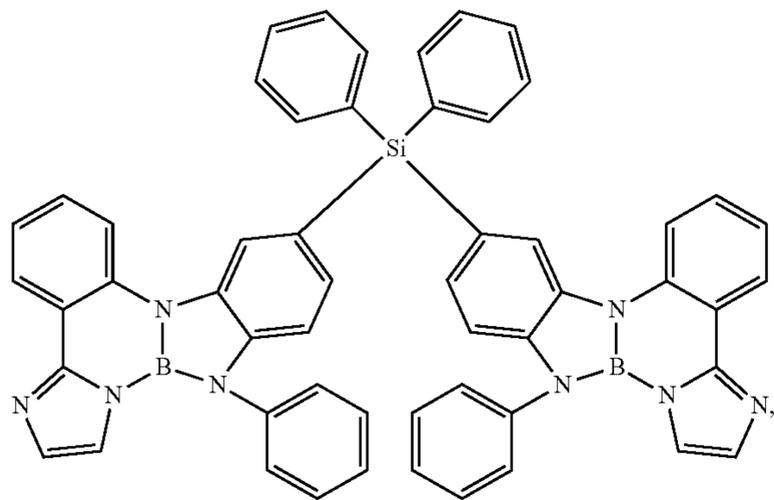
-continued



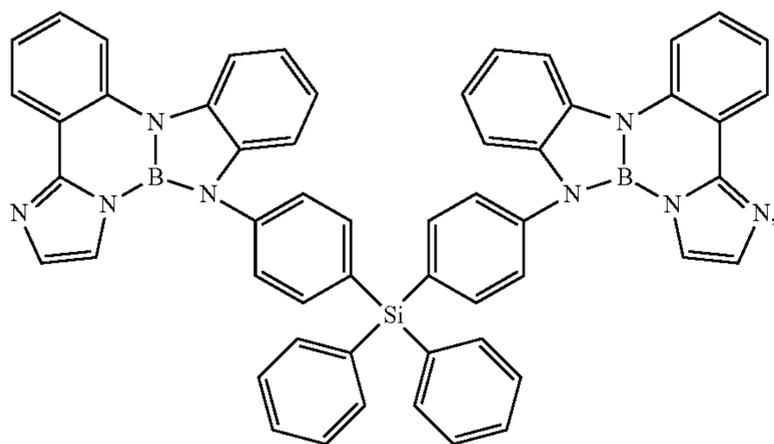
Compound 137



Compound 138



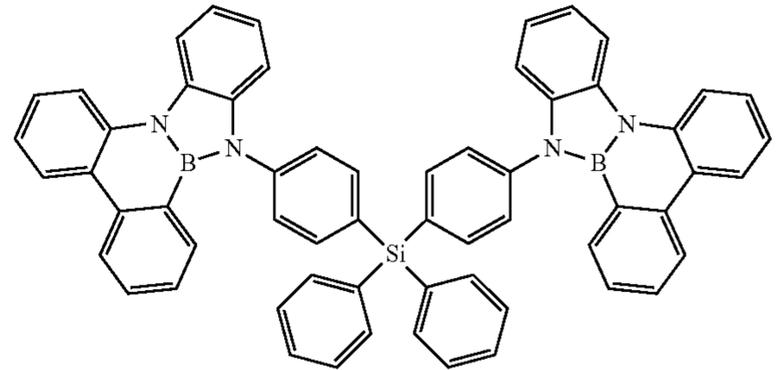
Compound 155



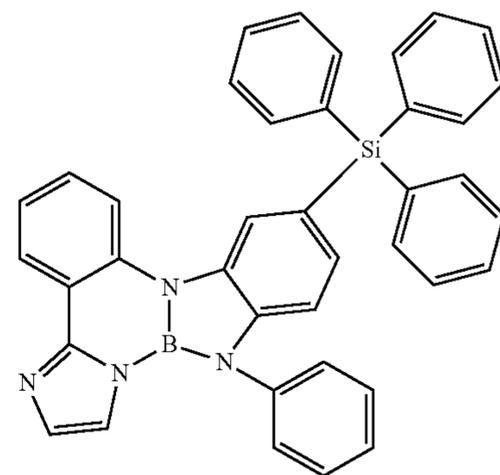
Compound 156

**182**

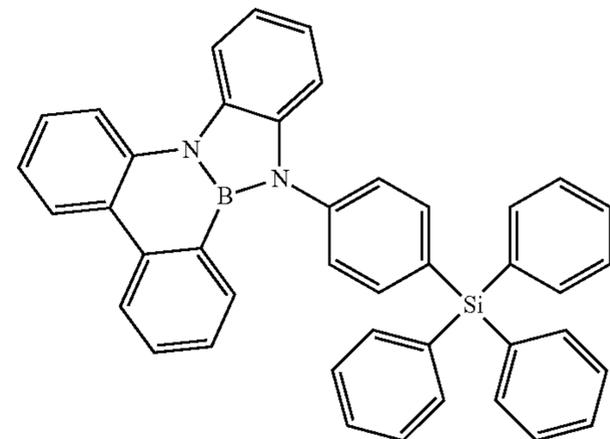
-continued



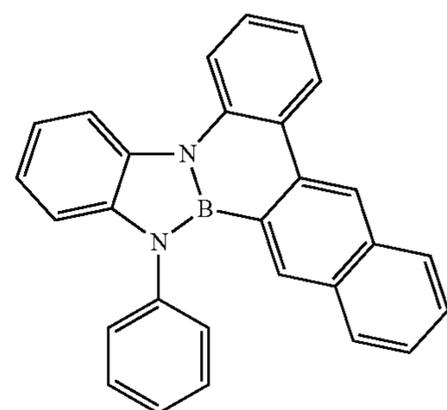
Compound 157



Compound 163



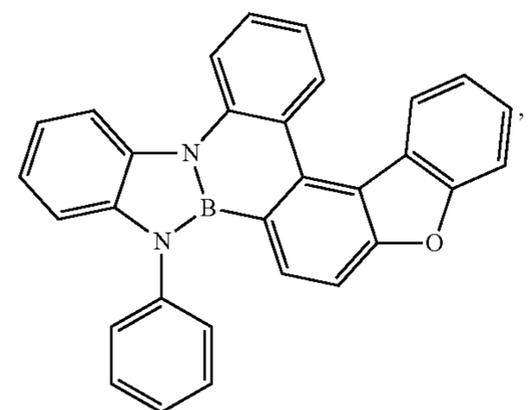
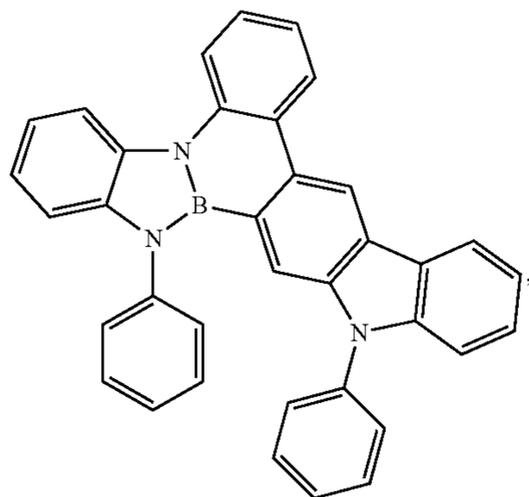
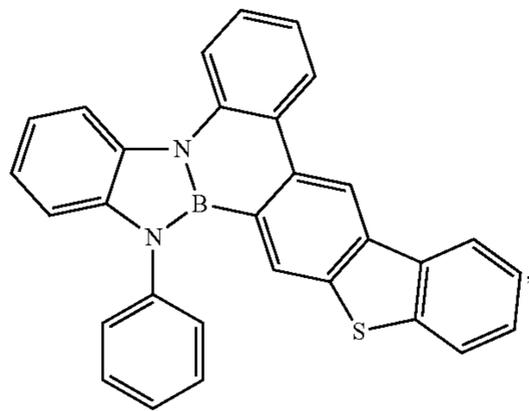
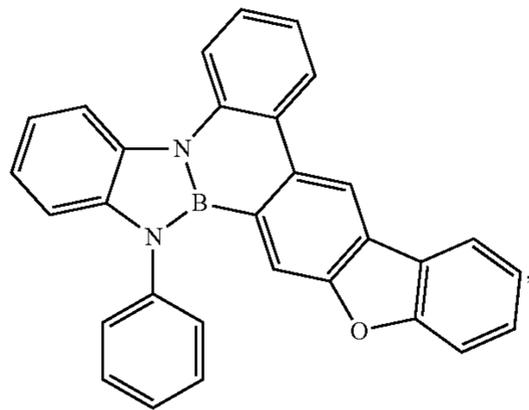
Compound 164



Compound 187

**183**

-continued



**184**

-continued

Compound 188

5

10

15

Compound 189

20

25

30

Compound 190

35

40

45

50

Compound 191

55

60

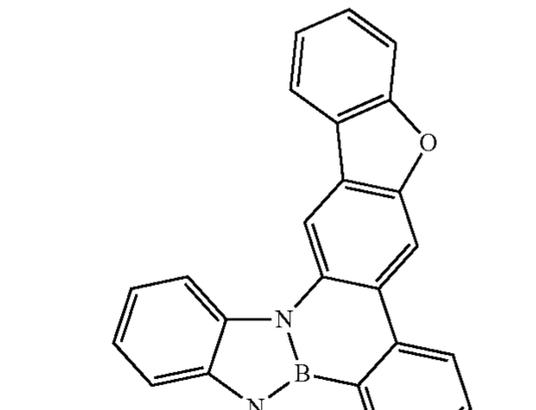
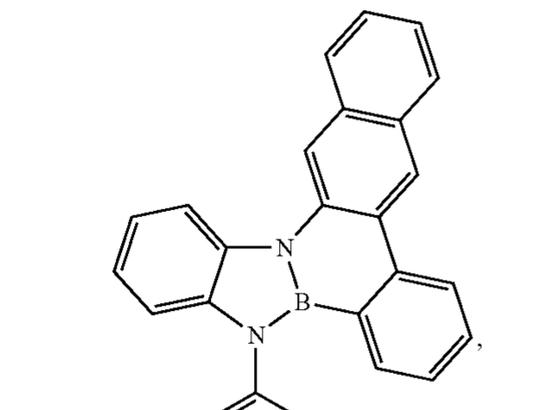
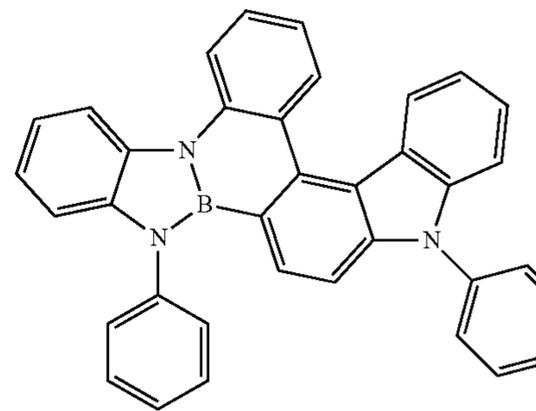
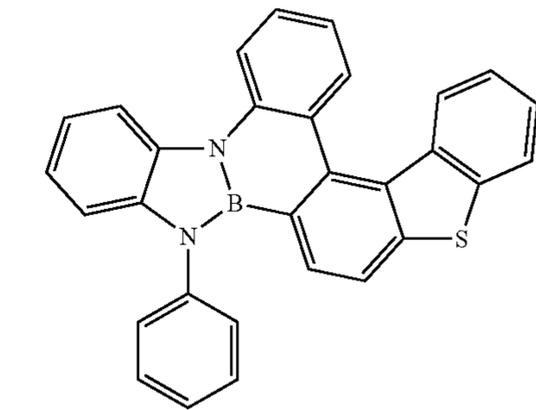
65

Compound 192

Compound 193

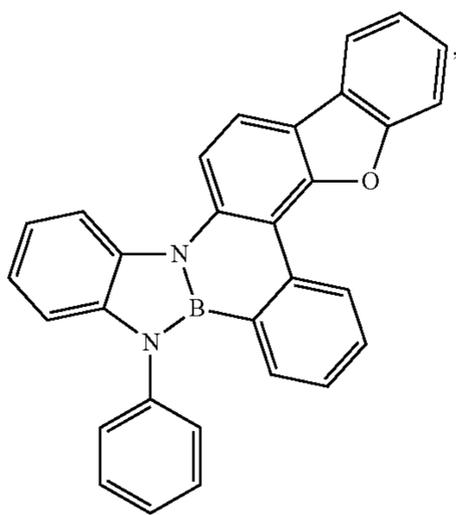
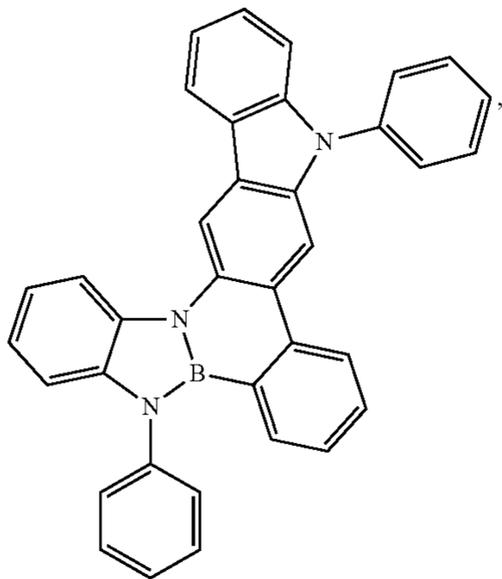
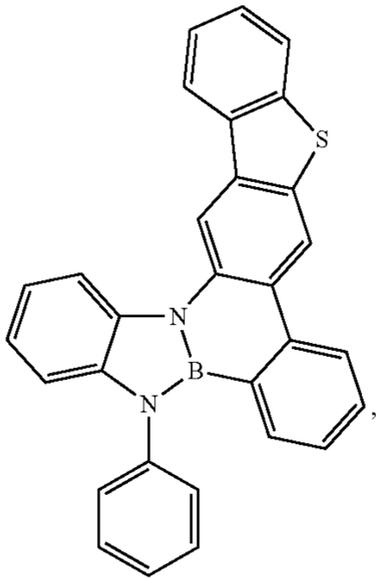
Compound 194

Compound 195



**185**

-continued



**186**

-continued

Compound 196

5

10

15

20

25

Compound 197

30

35

40

45

Compound 198

50

55

60

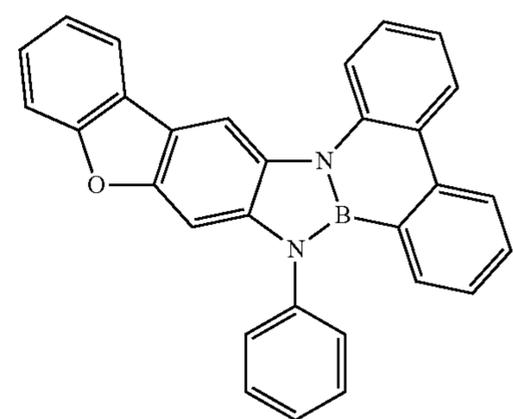
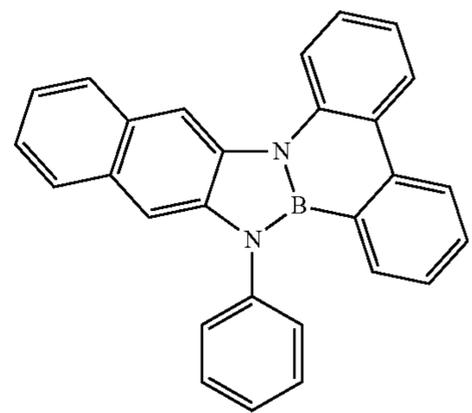
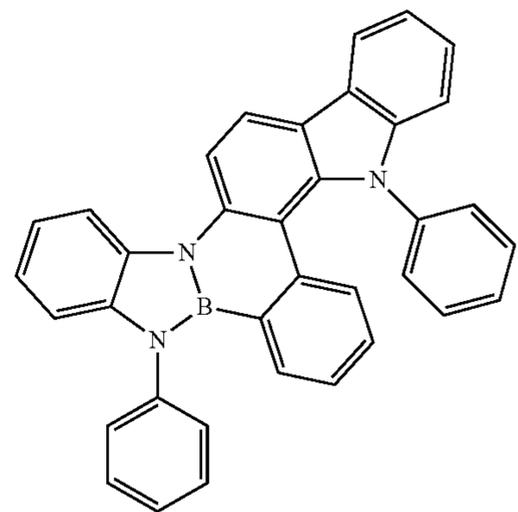
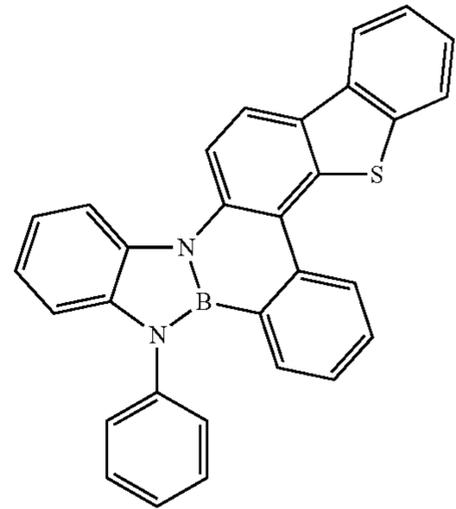
65

Compound 199

Compound 200

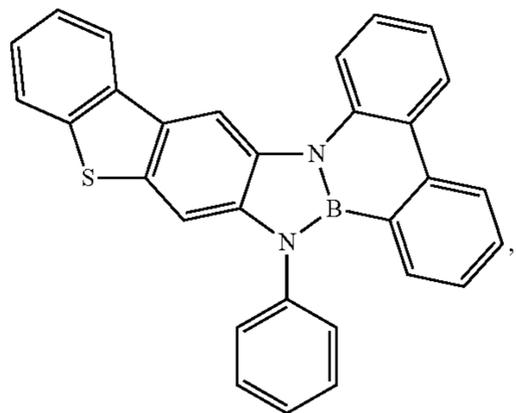
Compound 201

Compound 202



**187**

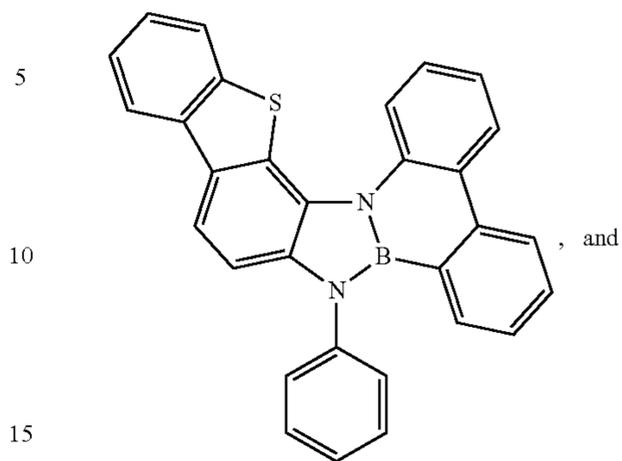
-continued



Compound 203

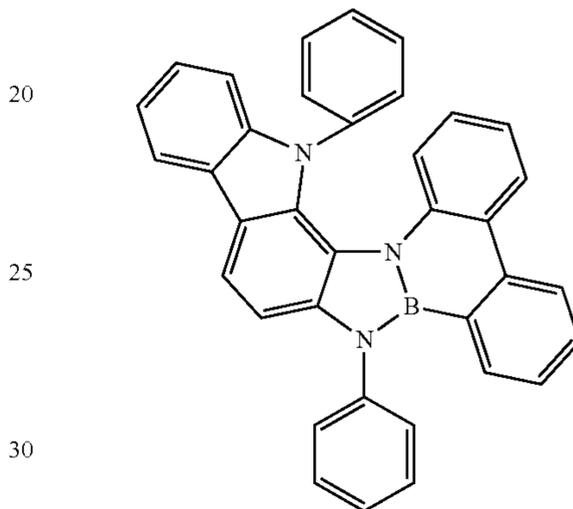
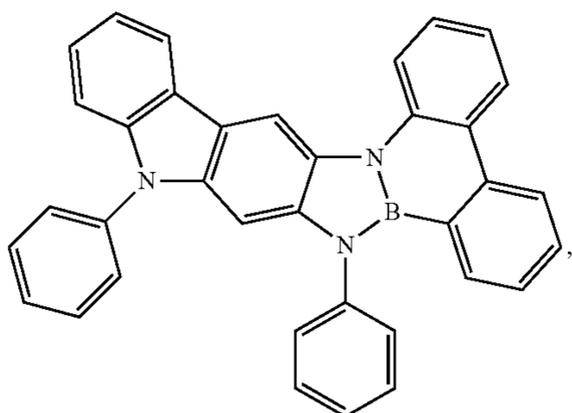
**188**

-continued



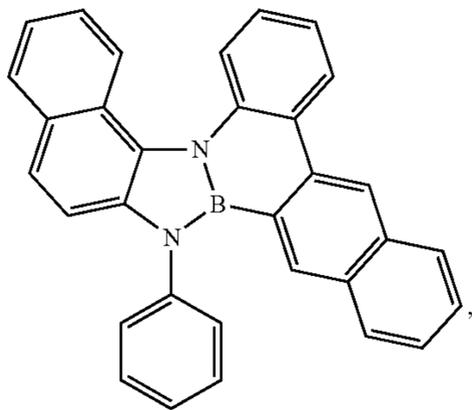
Compound 207

Compound 204



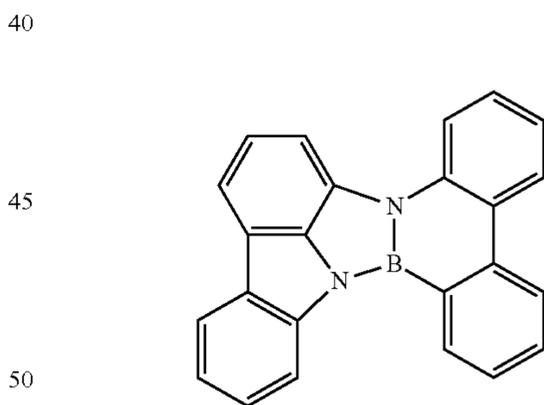
Compound 208

Compound 205



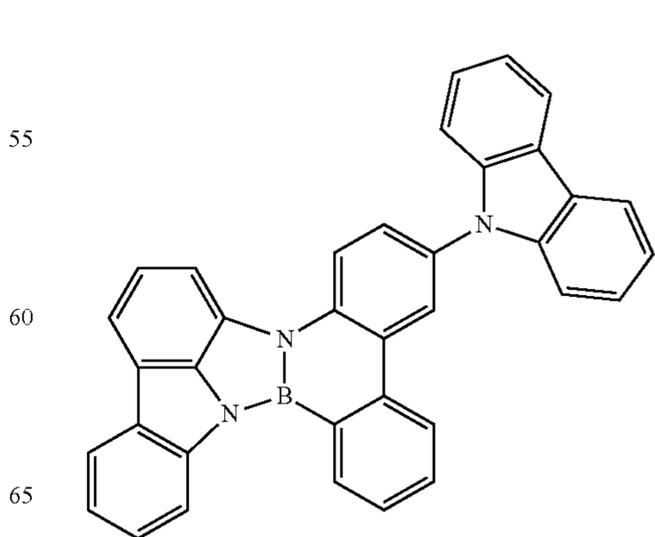
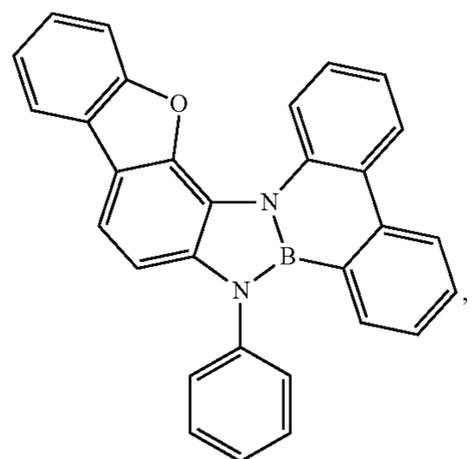
35 **5.** The compound of claim 1, wherein X<sup>1</sup> is C or N, A is aryl or heteroaryl and A is connected to X<sup>1</sup> to form a fused ring.

40 **6.** The compound of claim 5, wherein the compound is selected from the group consisting of:



Compound 1

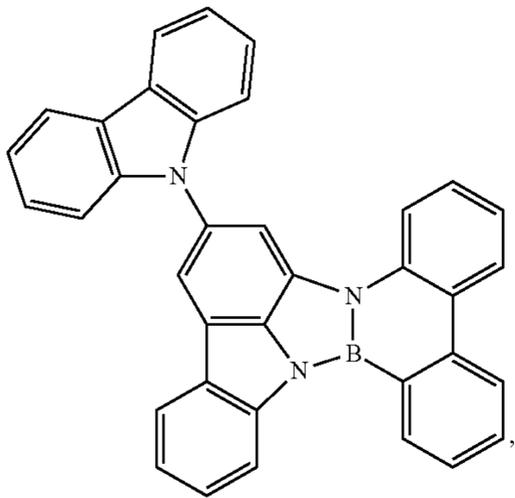
Compound 206



Compound 2

189

-continued



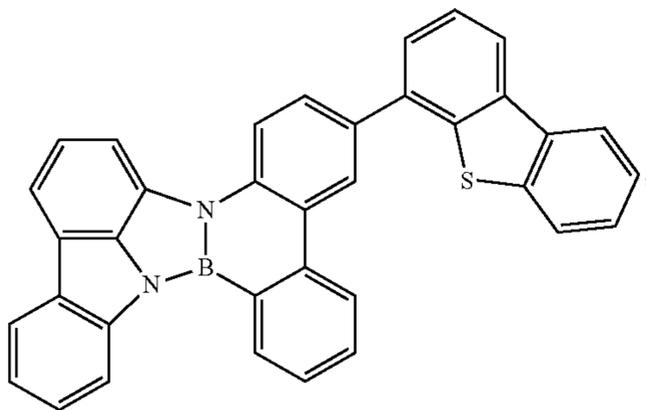
Compound 3

5

10

15

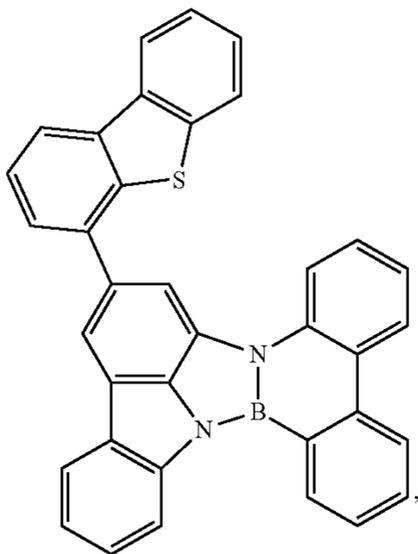
Compound 4



25

30

Compound 5



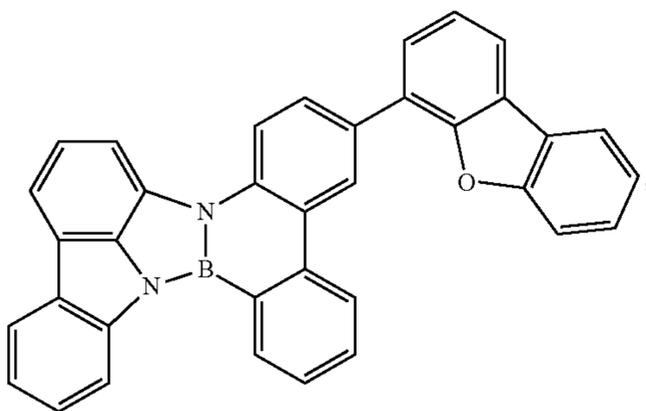
35

40

45

50

Compound 6



55

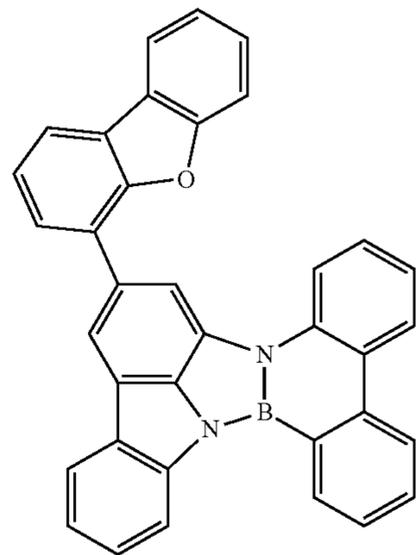
60

65

190

-continued

Compound 7

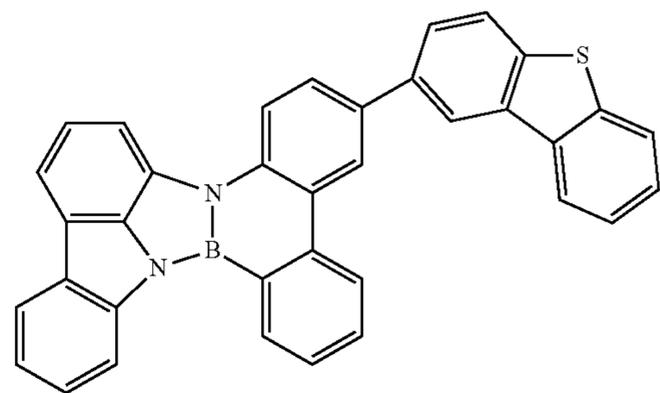


5

10

15

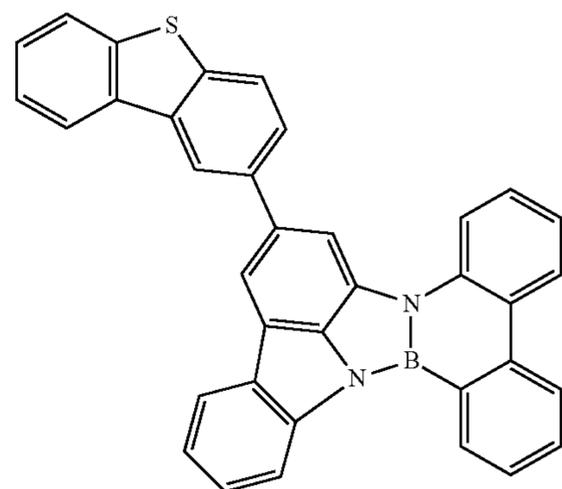
Compound 8



25

30

Compound 9



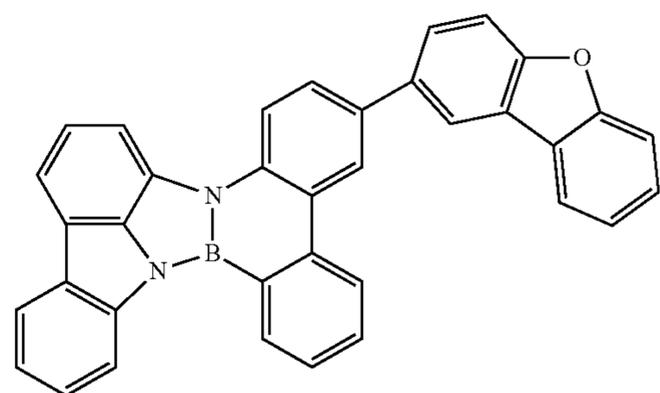
35

40

45

50

Compound 10



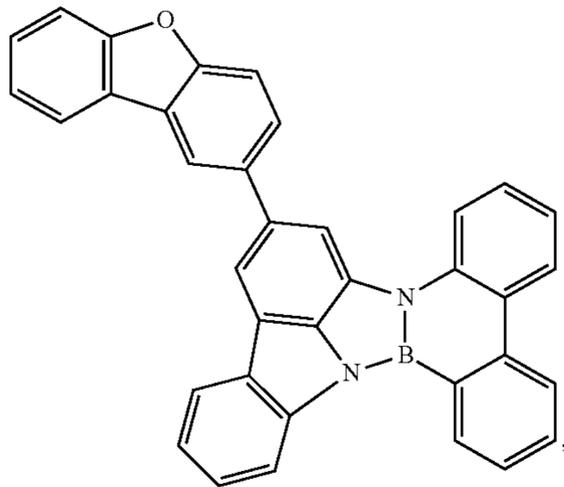
55

60

65

191

-continued

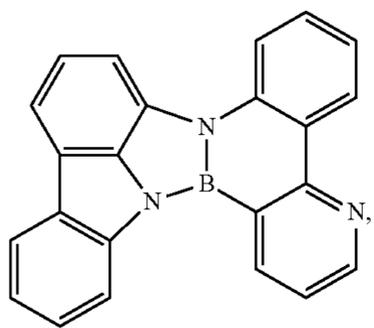


Compound 11

5

10

15

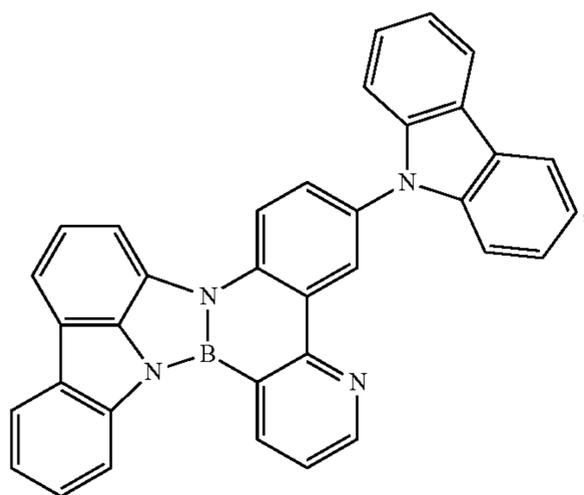


Compound 12

20

25

30



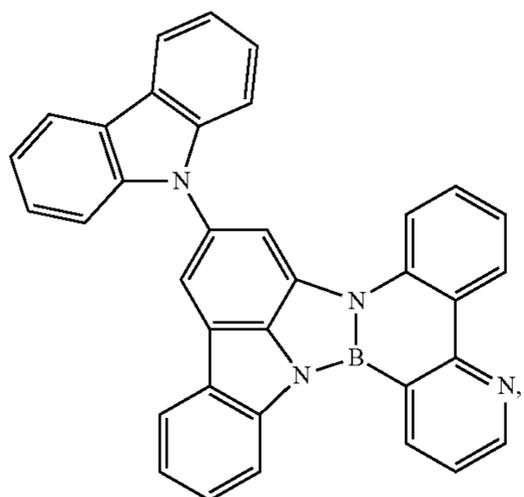
Compound 13

35

40

45

50



Compound 14

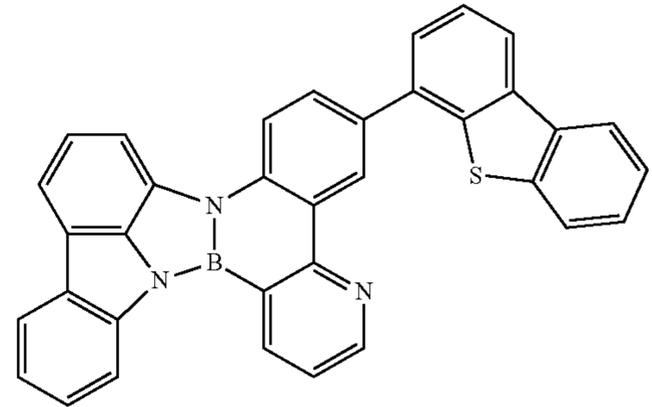
55

60

65

192

-continued

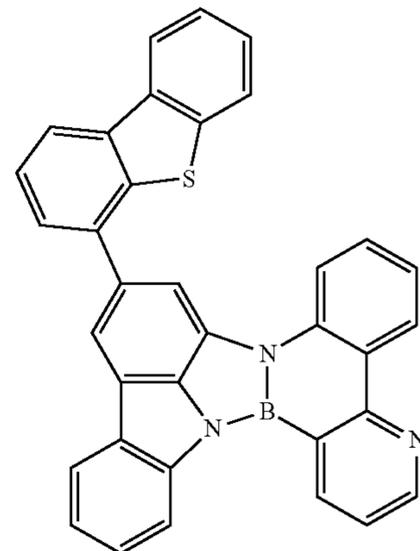


Compound 15

5

10

15

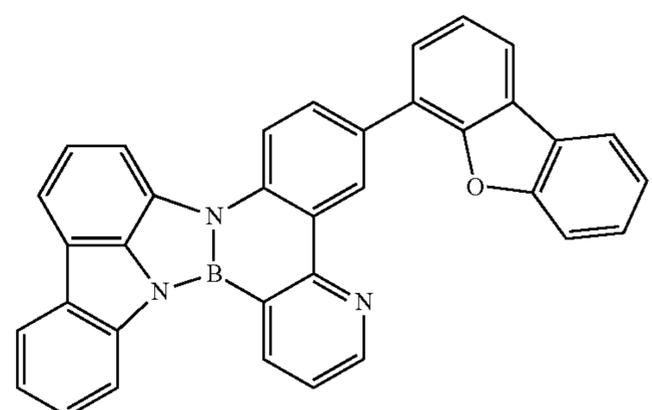


Compound 16

20

25

30



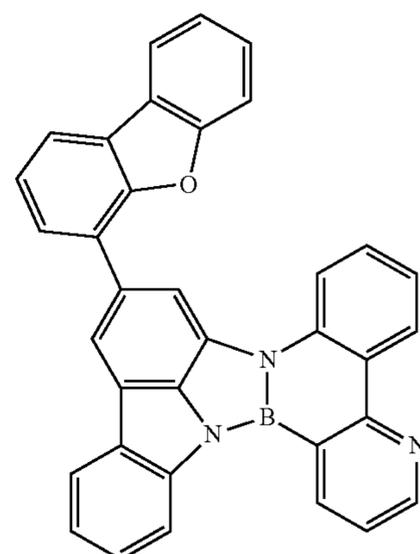
Compound 17

35

40

45

50



Compound 18

55

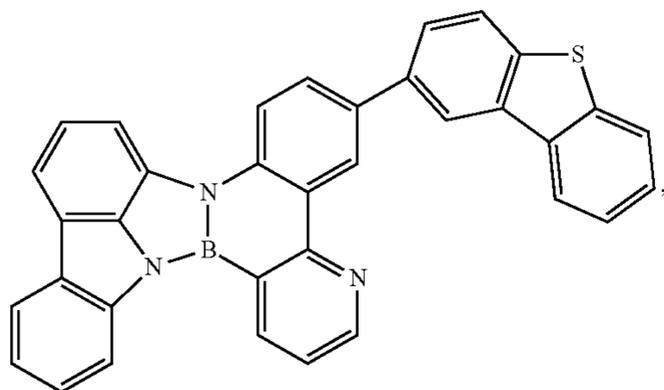
60

65

193

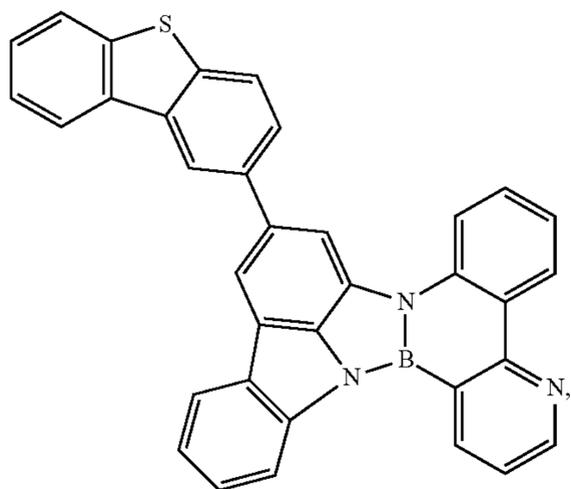
-continued

Compound 19



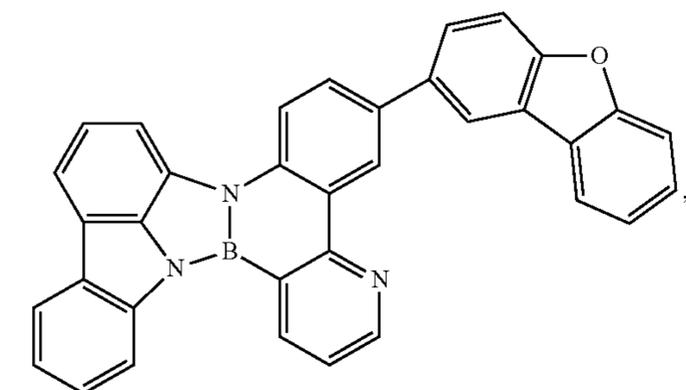
5

Compound 20



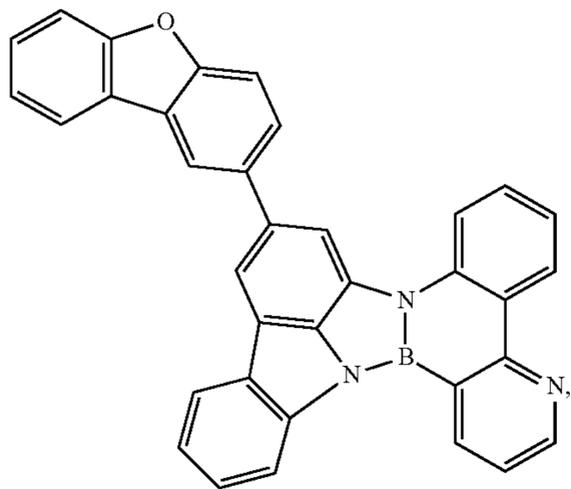
15

Compound 21



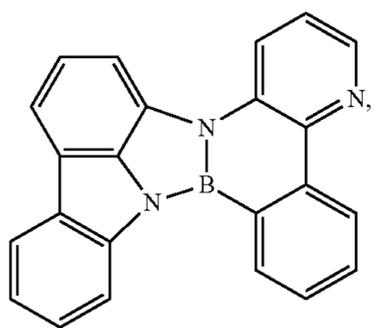
35

Compound 22



45

Compound 23

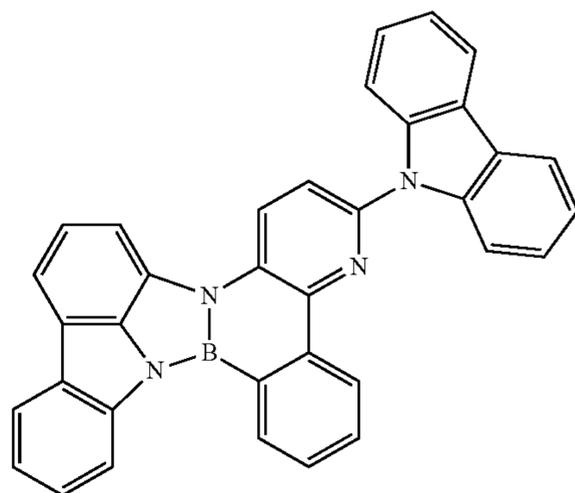


65

194

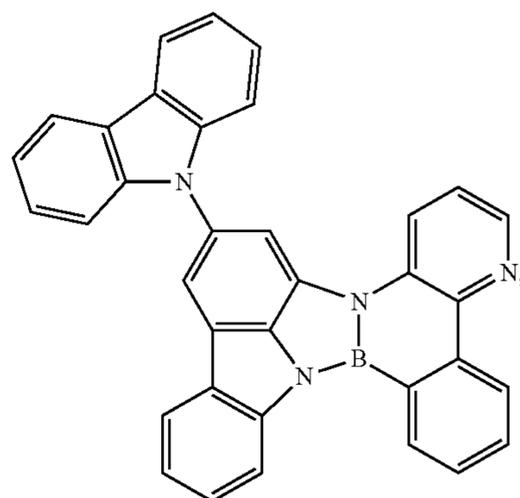
-continued

Compound 24



10

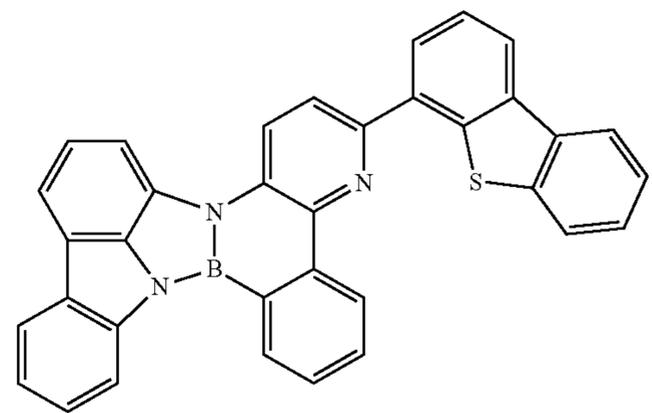
Compound 25



20

25

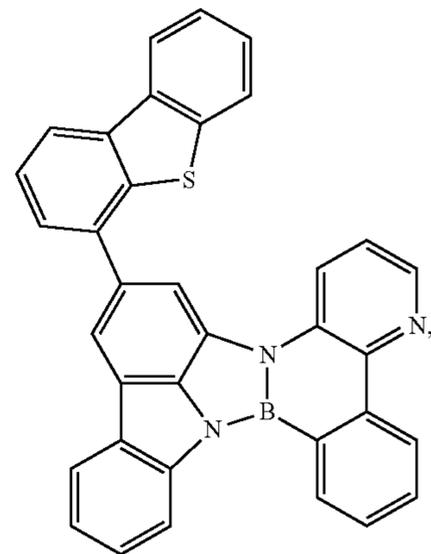
Compound 26



40

45

Compound 27



50

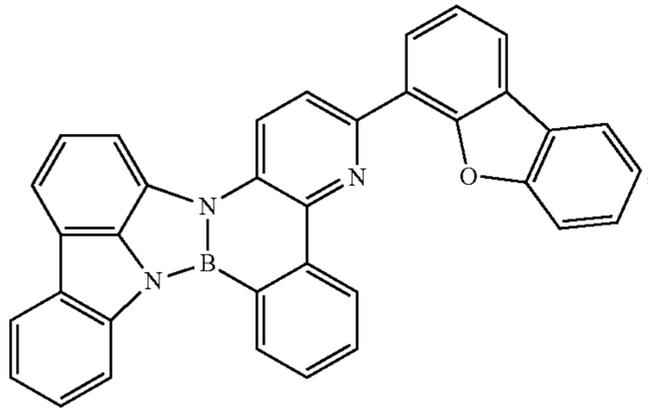
55

60

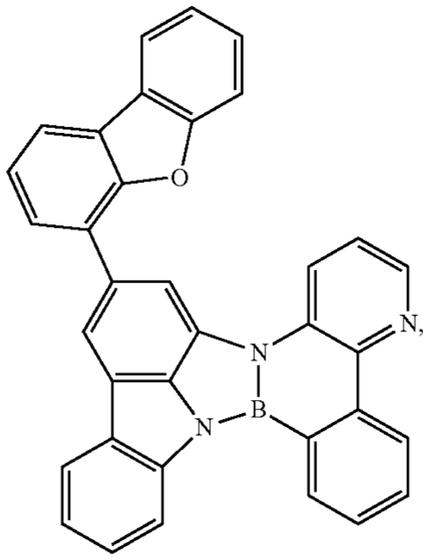
195

-continued

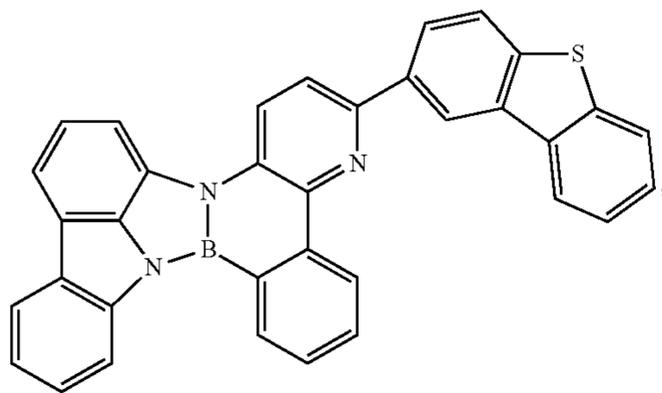
Compound 28



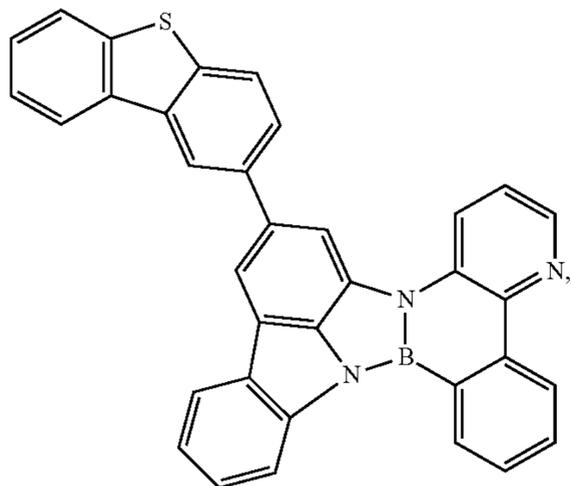
Compound 29



Compound 30



Compound 31

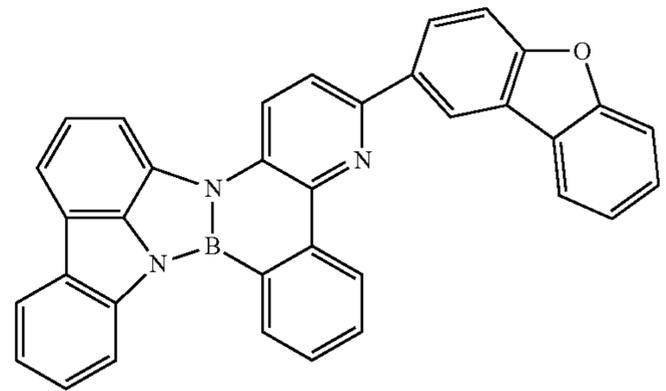


196

-continued

Compound 32

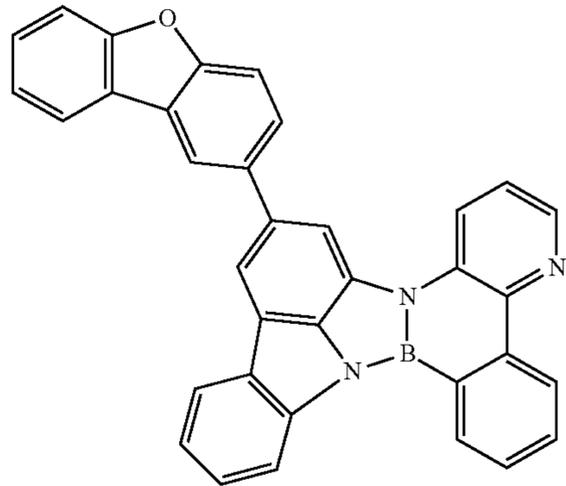
5



10

15

Compound 33



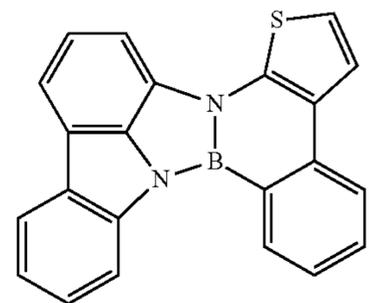
20

25

30

Compound 49

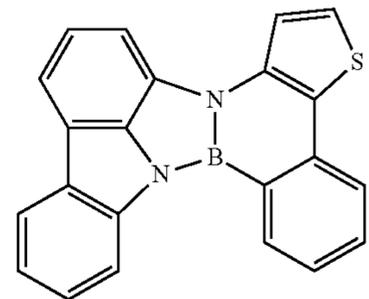
35



40

45

Compound 50

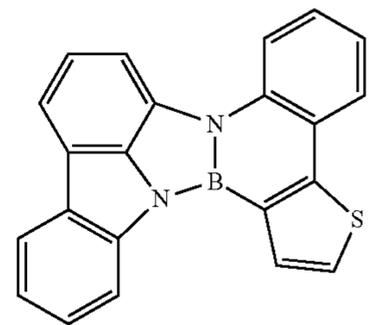


50

55

Compound 51

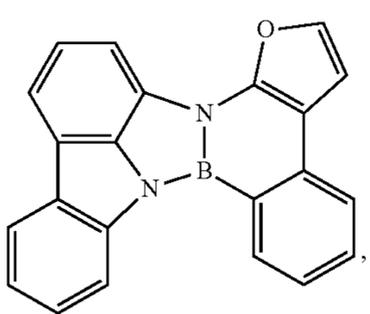
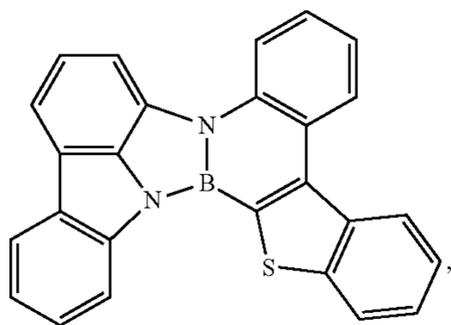
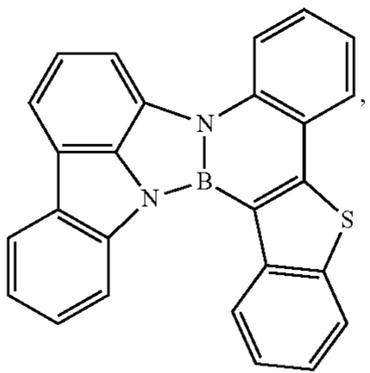
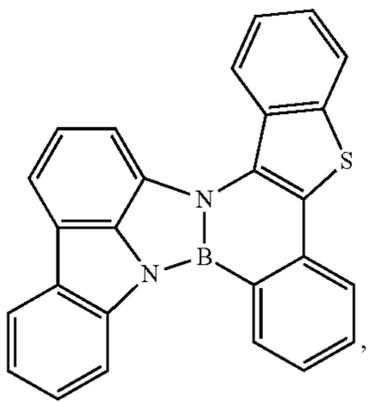
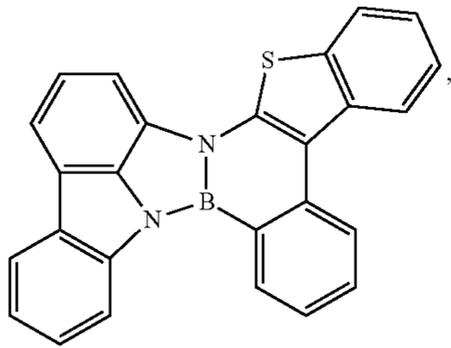
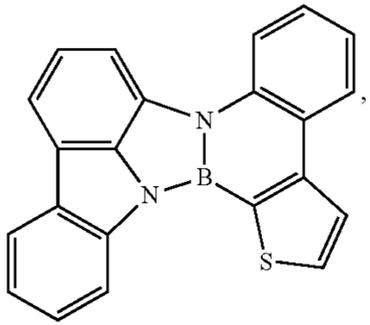
60



65

**197**

-continued

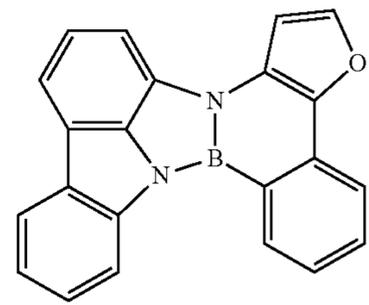


**198**

-continued

Compound 52

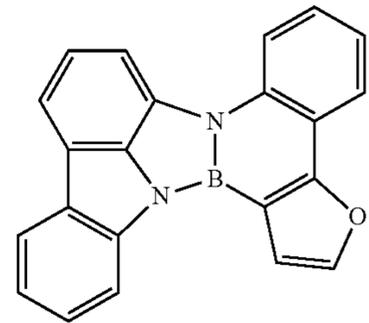
5



10

Compound 53

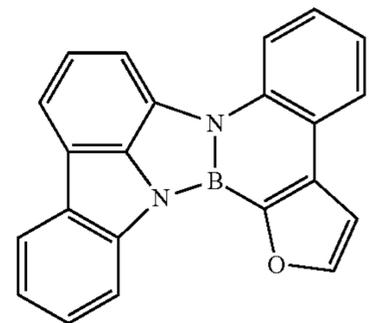
15



20

Compound 54

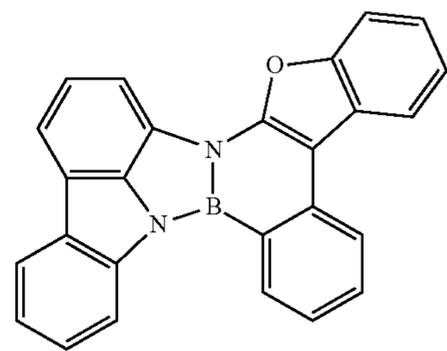
25



30

Compound 55

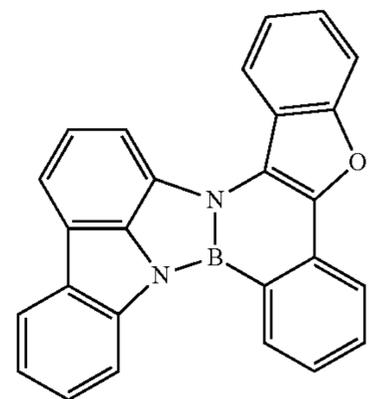
35



40

Compound 56

45

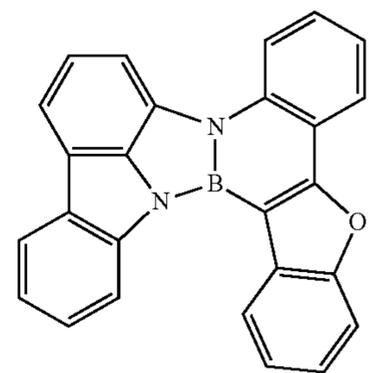


50

55

Compound 57

60



65

Compound 58

Compound 59

Compound 60

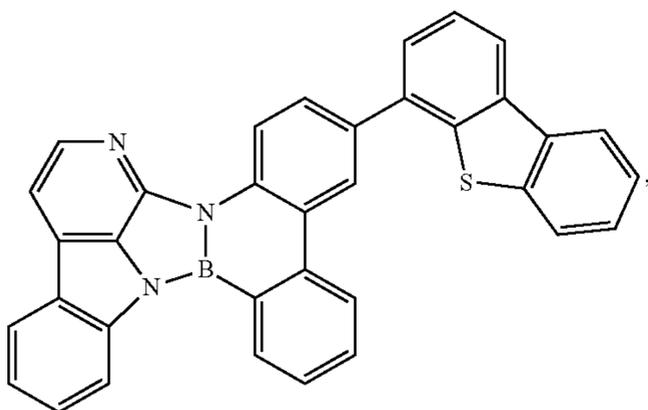
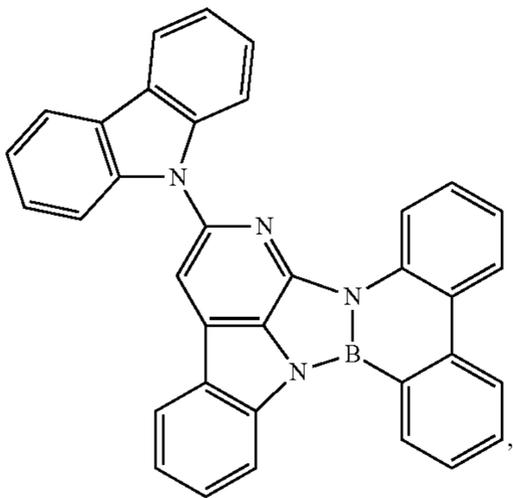
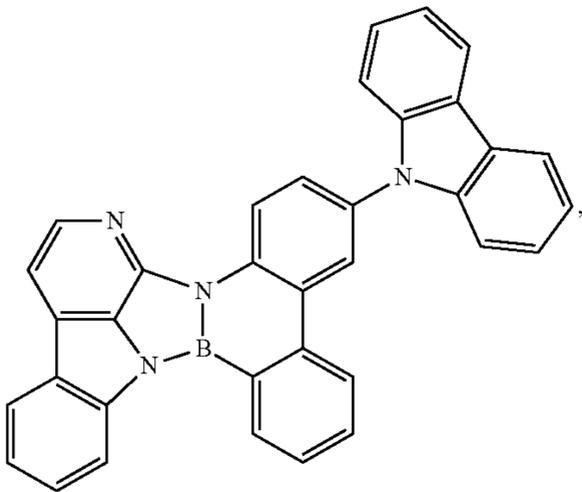
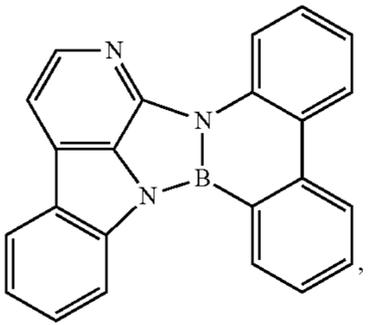
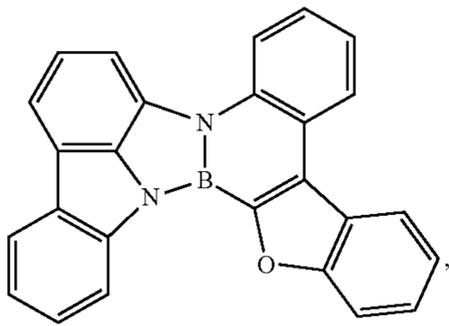
Compound 61

Compound 62

Compound 63

**199**

-continued



**200**

-continued

Compound 64

5

10

Compound 65

15

20

Compound 66

25

30

35

Compound 67

40

45

50

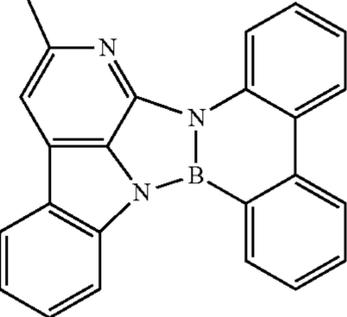
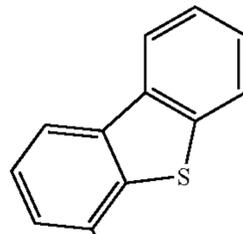
55

Compound 68

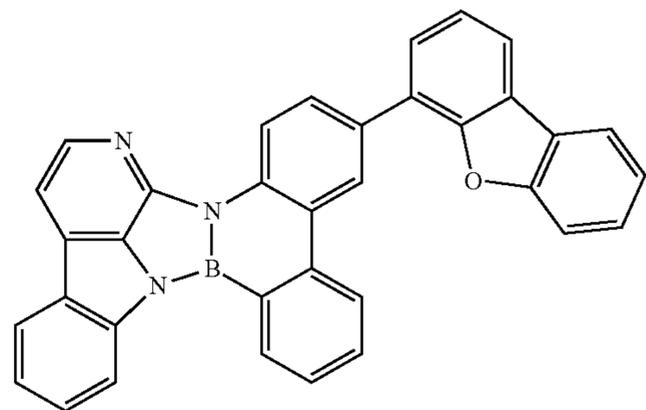
60

65

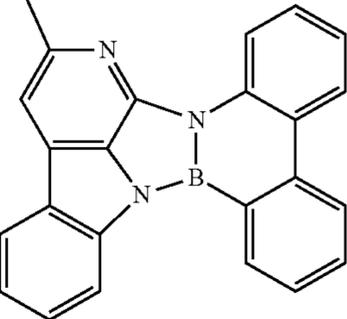
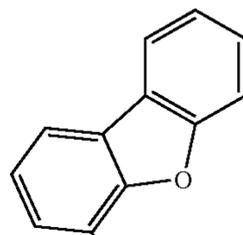
Compound 69



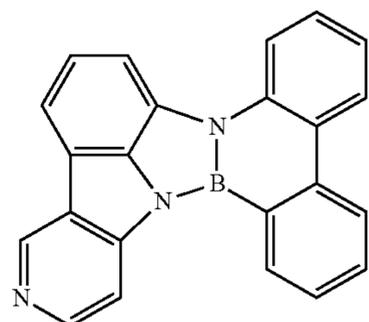
Compound 70



Compound 71



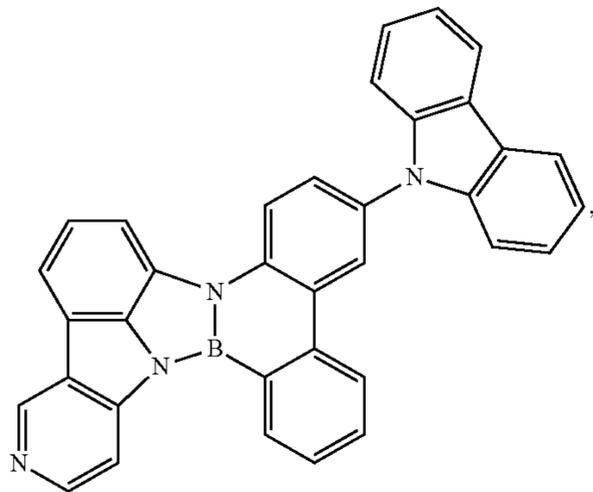
Compound 72



201

-continued

Compound 73

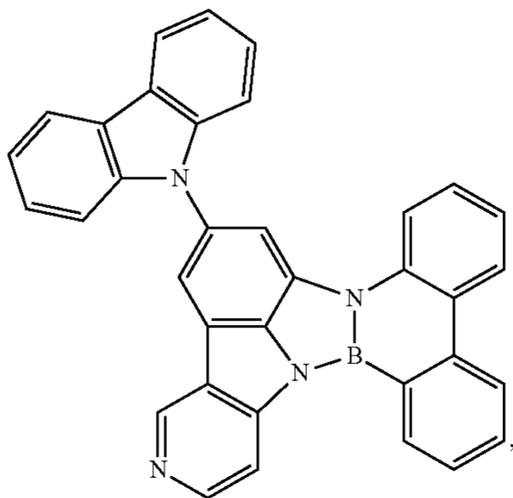


5

10

15

Compound 74

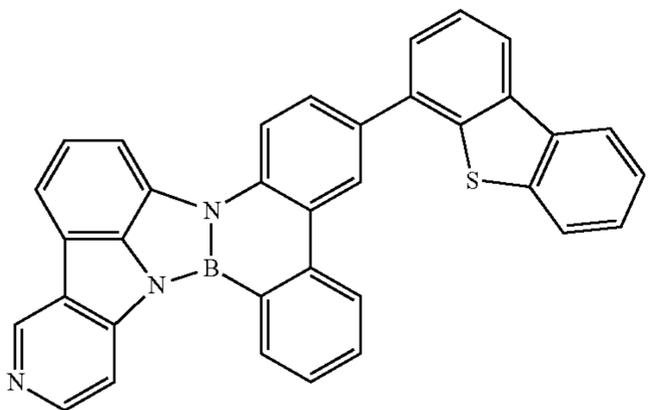


20

25

30

Compound 75

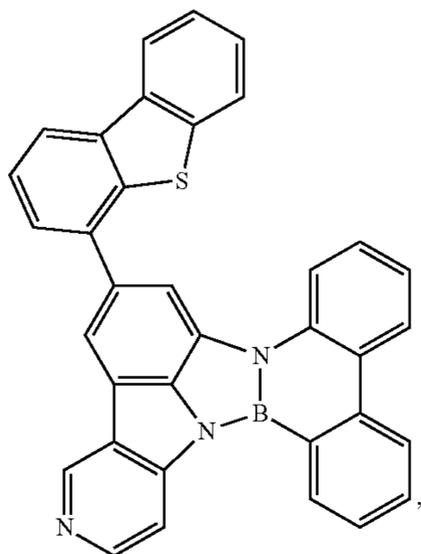


35

40

45

Compound 76



50

55

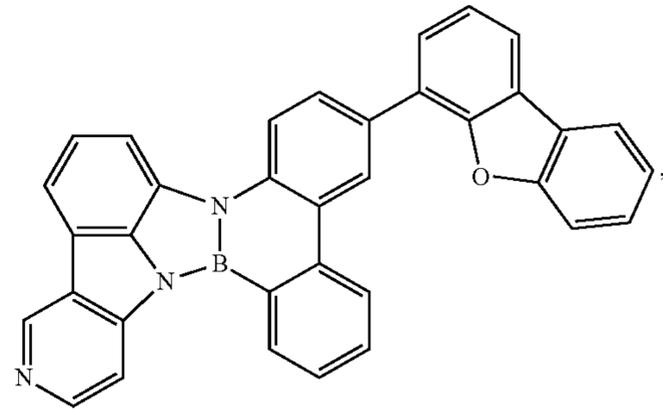
60

65

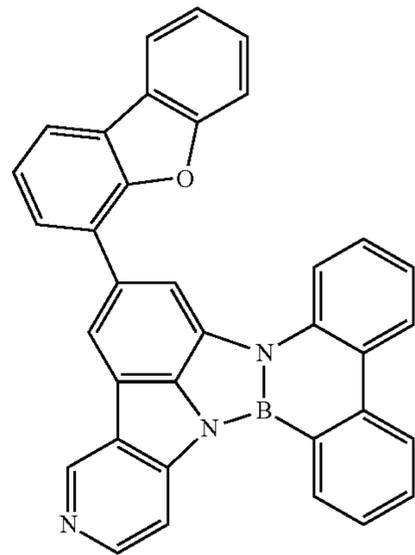
202

-continued

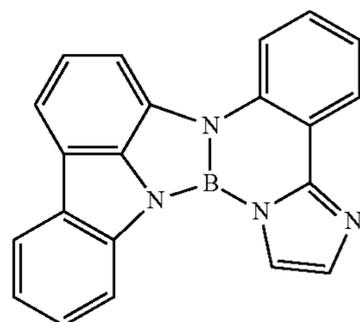
Compound 77



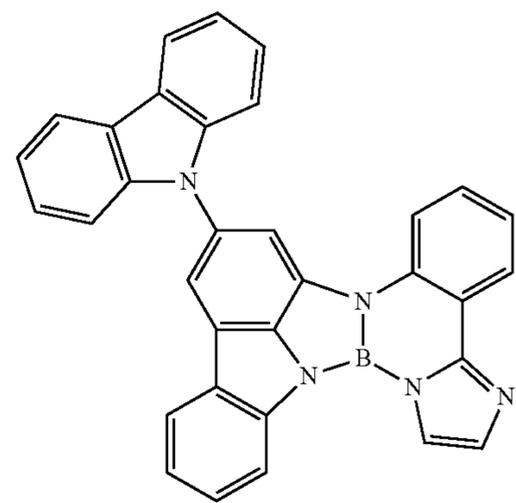
Compound 78



Compound 139

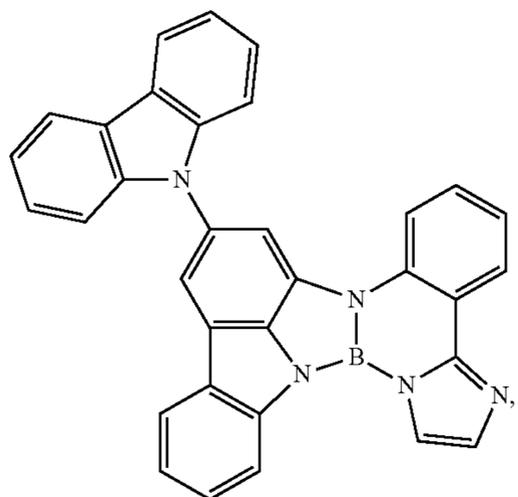


Compound 140



203

-continued

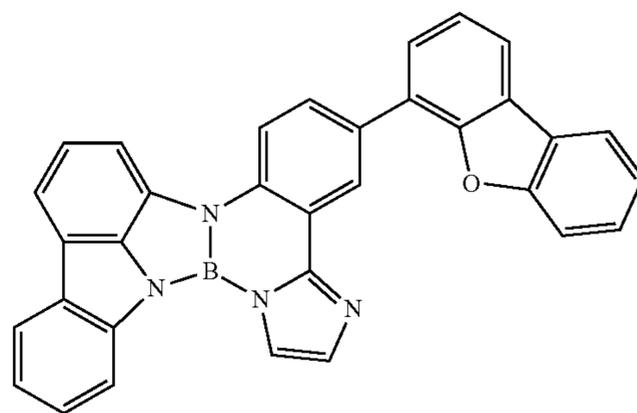


Compound 141

5

204

-continued



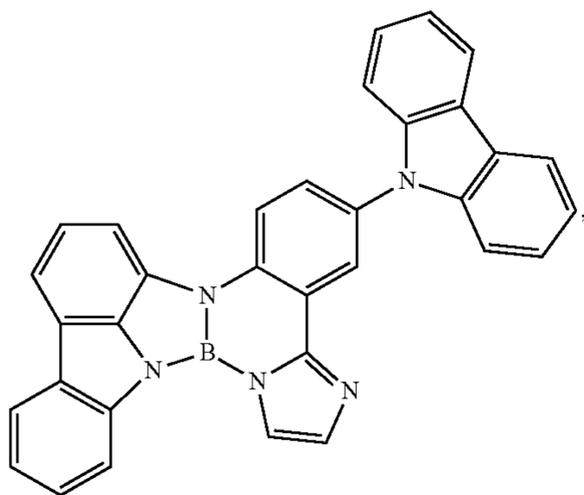
Compound 145

10

15

Compound 146

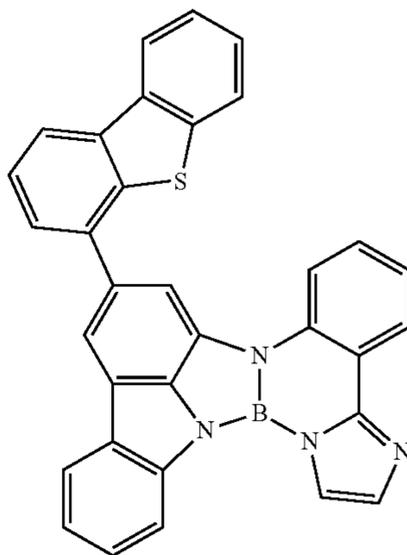
Compound 142



20

25

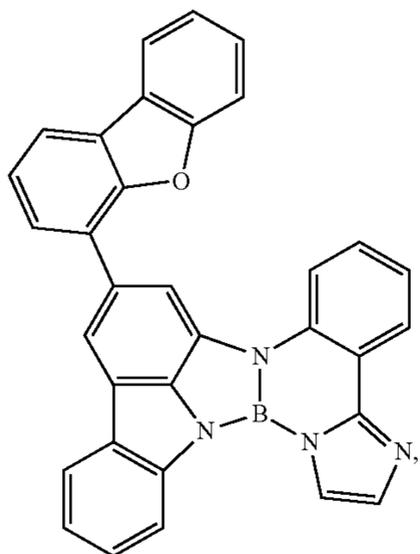
30



Compound 143

35

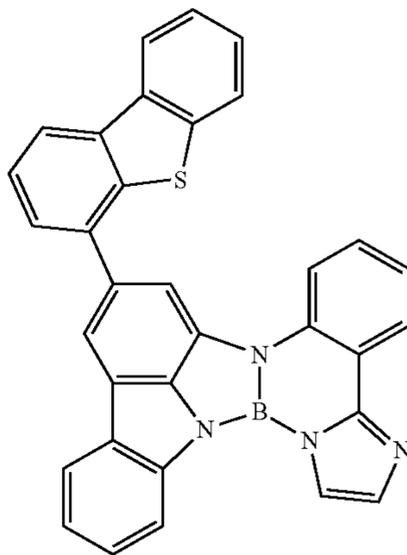
Compound 147



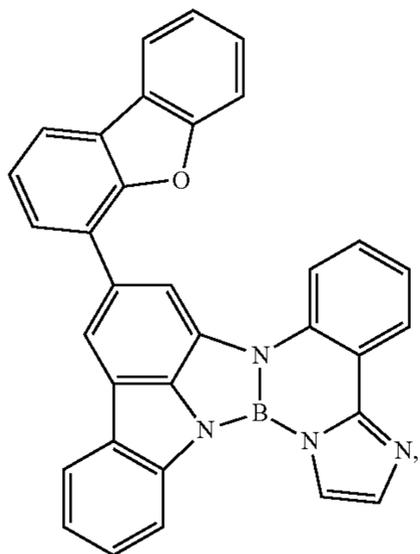
40

45

50



Compound 144

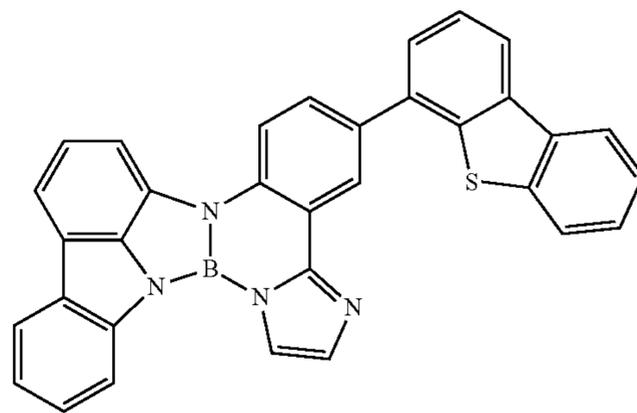


55

Compound 148

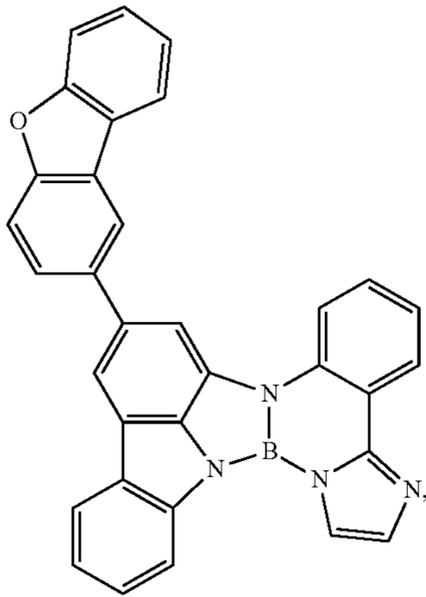
60

65



**205**

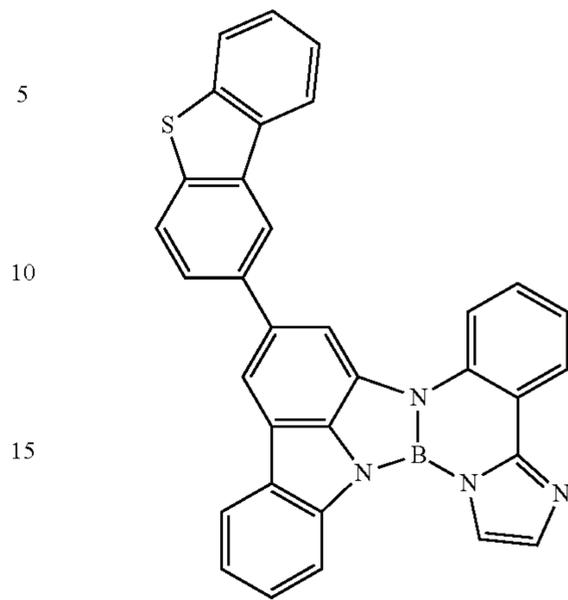
-continued



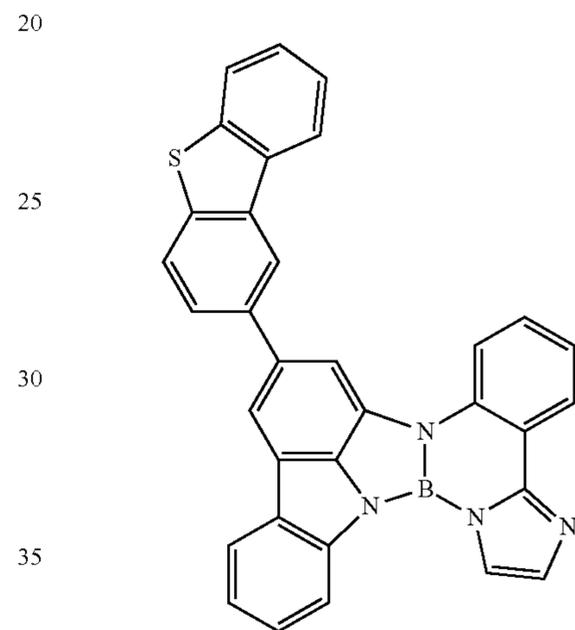
Compound 149

**206**

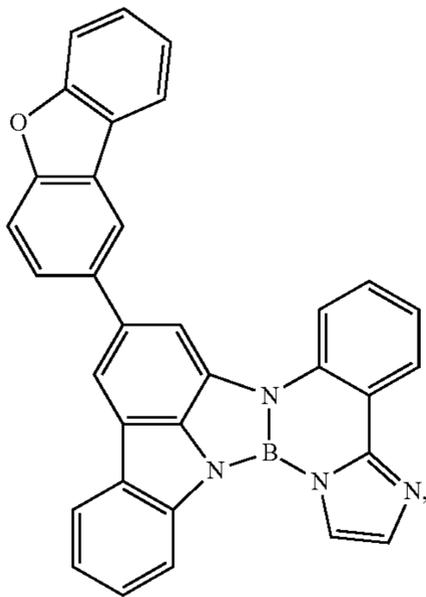
-continued



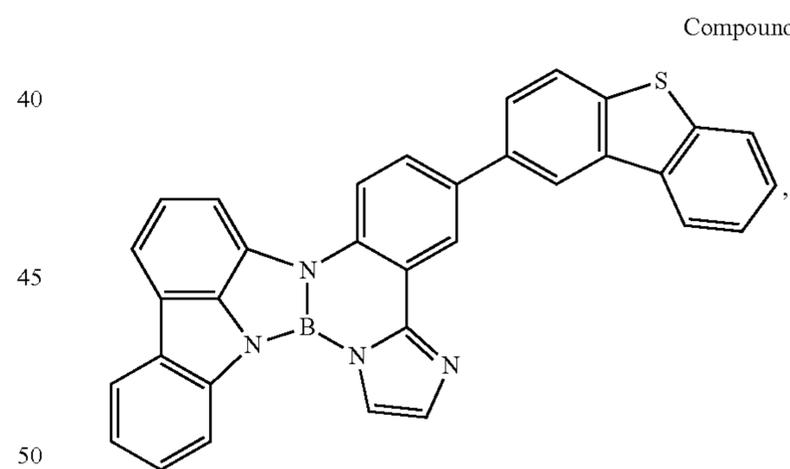
Compound 152



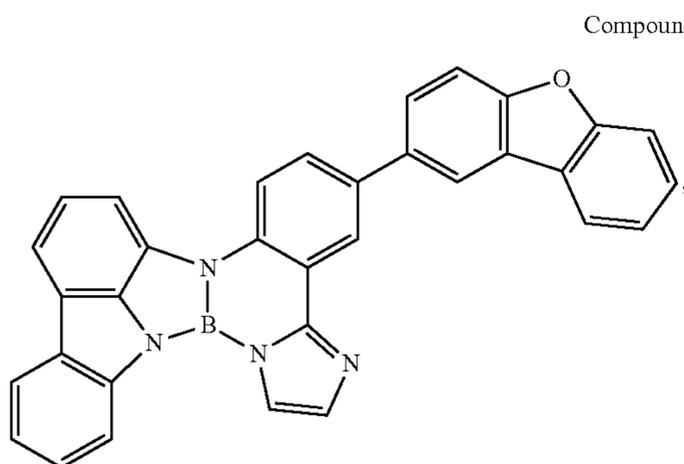
Compound 153



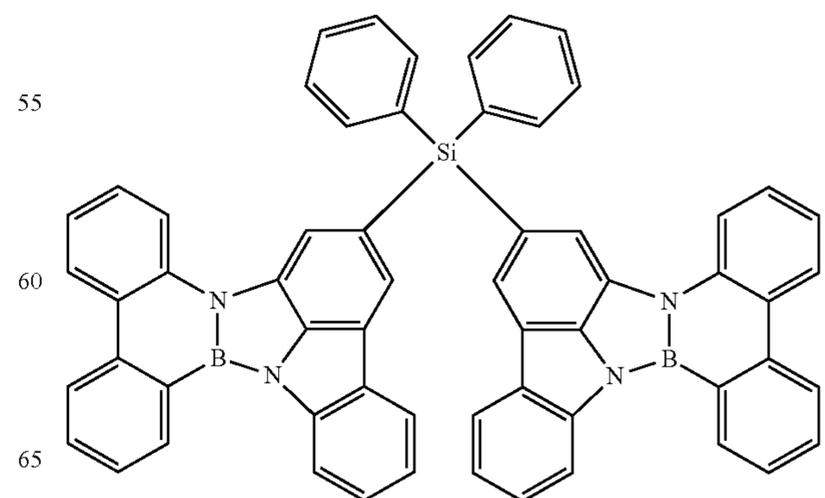
Compound 150



Compound 154



Compound 151

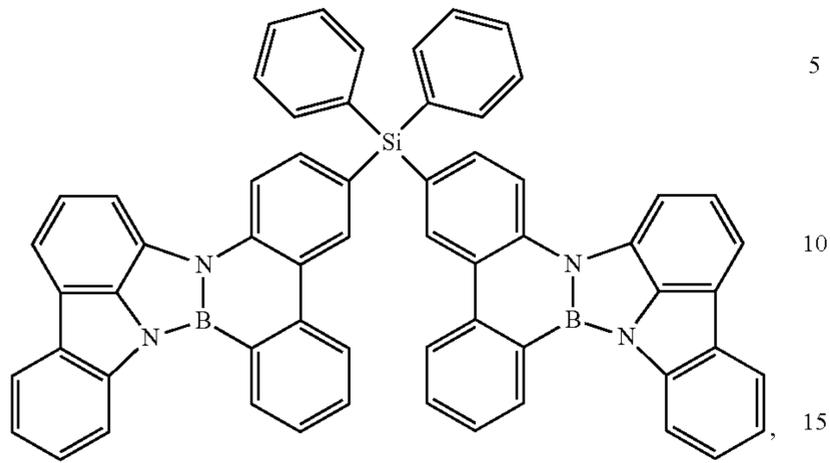


Compound 159

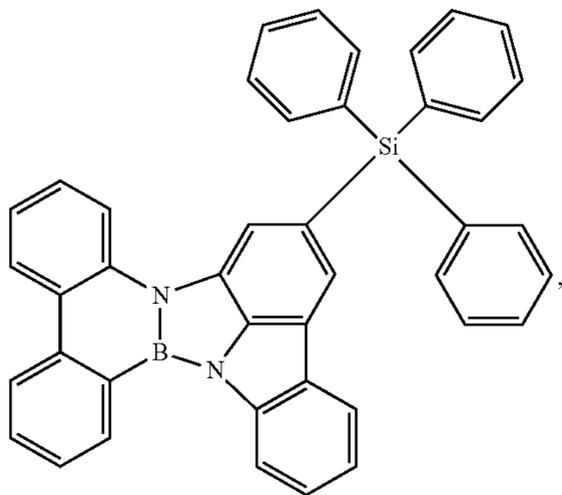
207

-continued

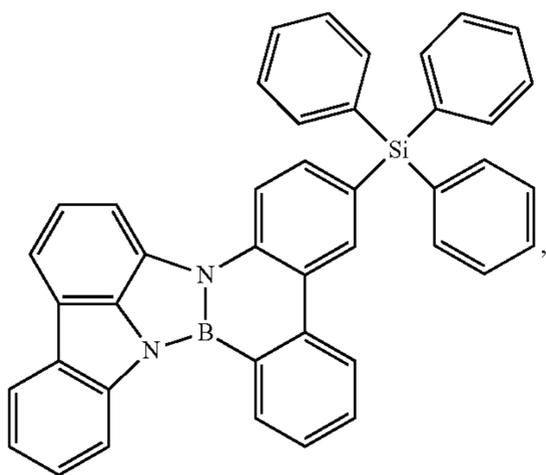
Compound 160



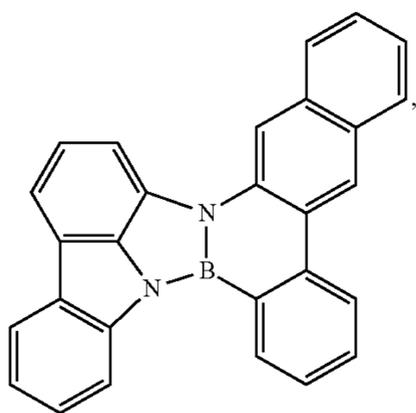
Compound 161



Compound 162



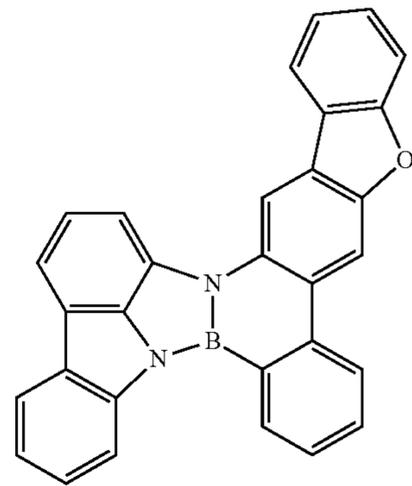
Compound 165



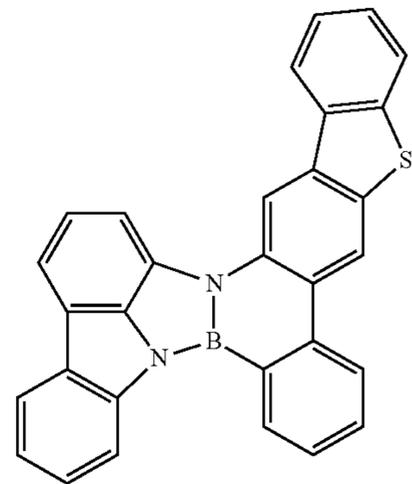
208

-continued

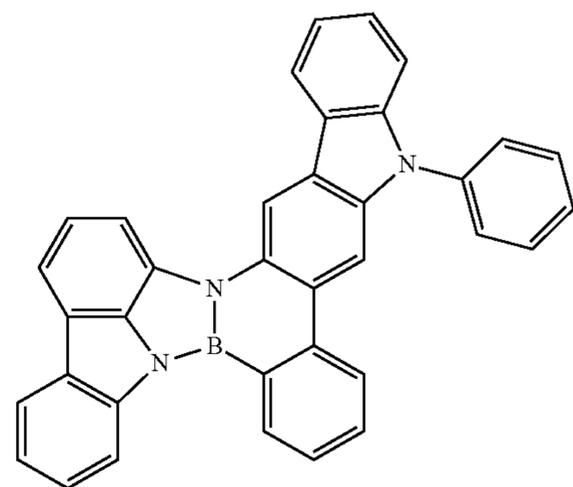
Compound 166



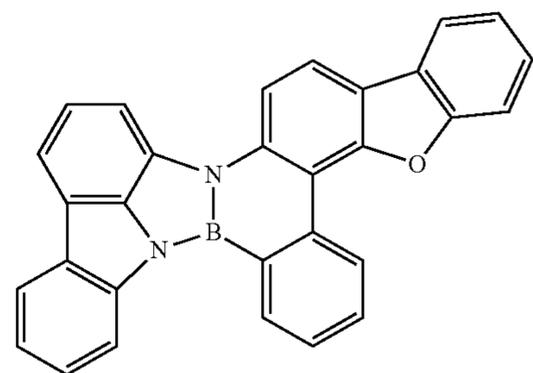
Compound 167



Compound 168

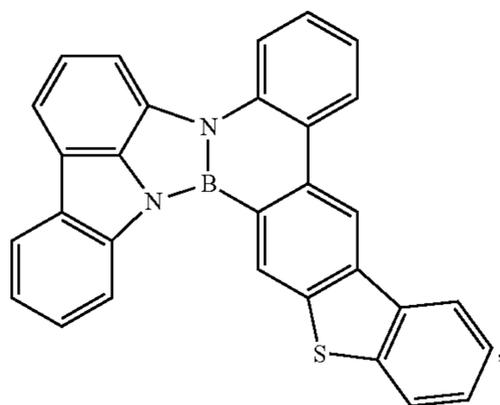
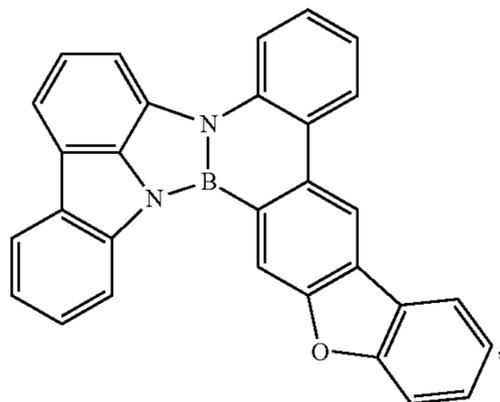
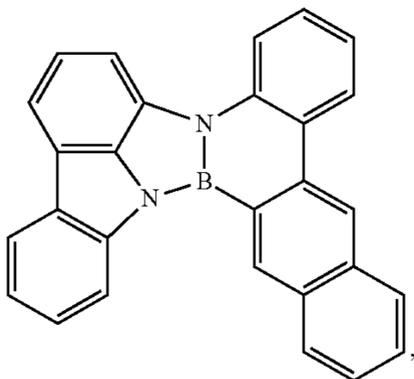
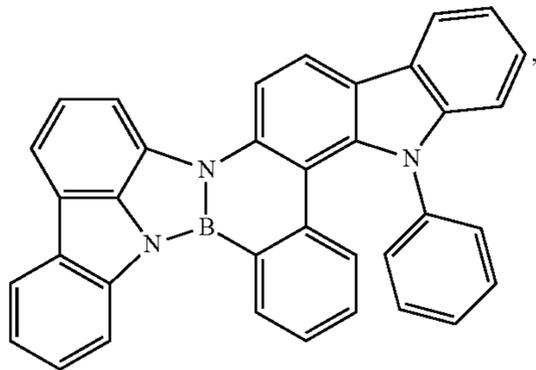
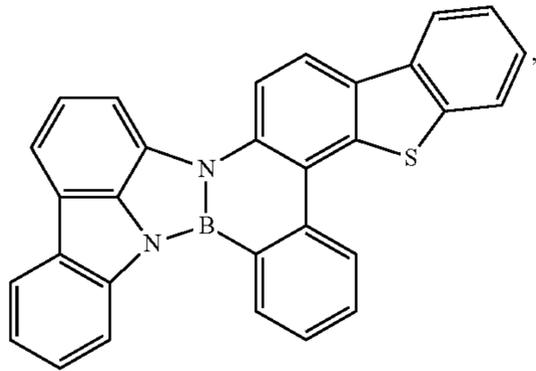


Compound 169



**209**

-continued

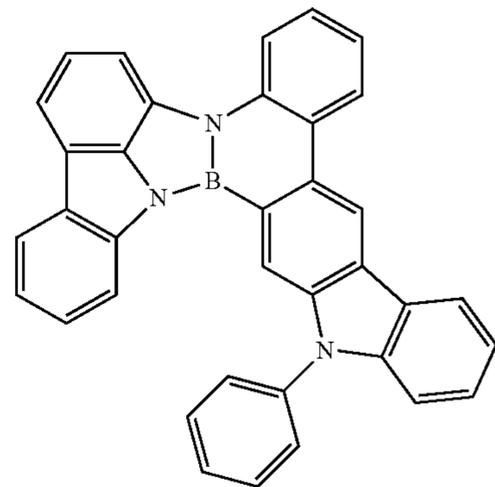


**210**

-continued

Compound 170

5



Compound 171

15

20

25

Compound 172

30

35

Compound 173

40

45

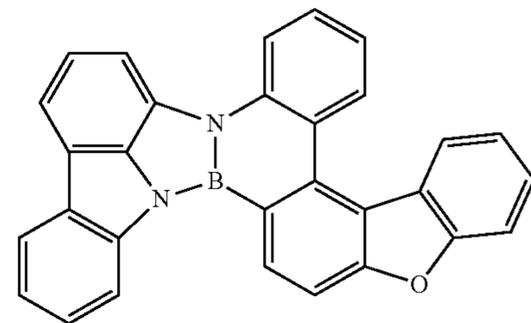
50

Compound 174

55

60

65



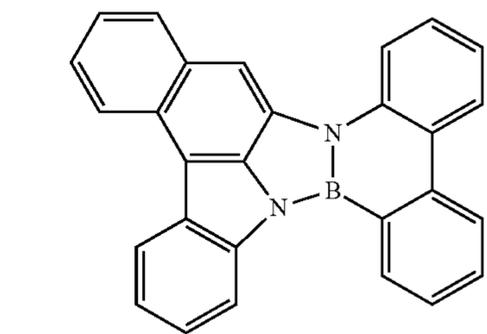
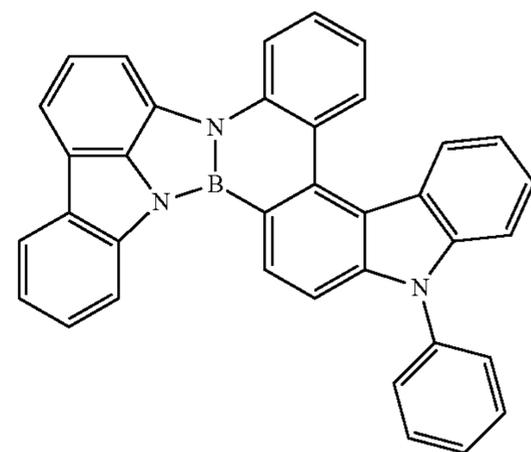
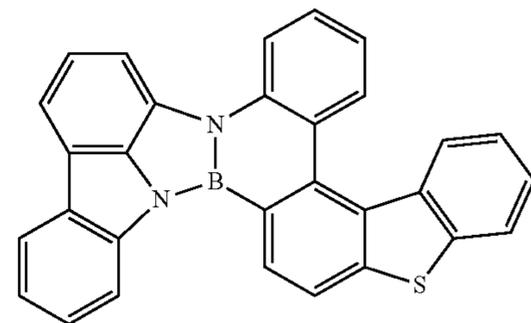
Compound 175

Compound 176

Compound 177

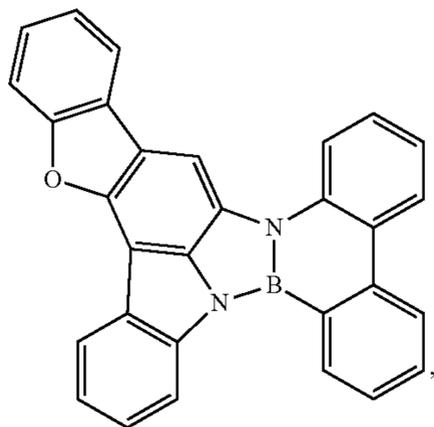
Compound 178

Compound 179



211

-continued



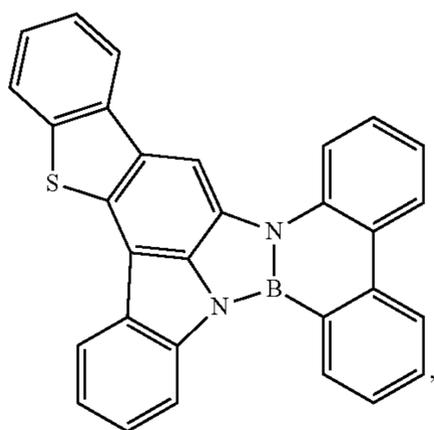
Compound 180

5

10

15

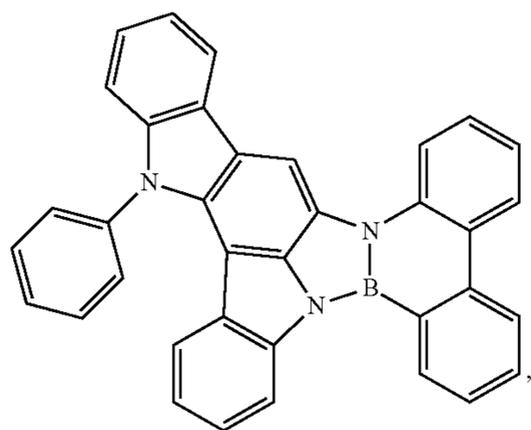
Compound 181



25

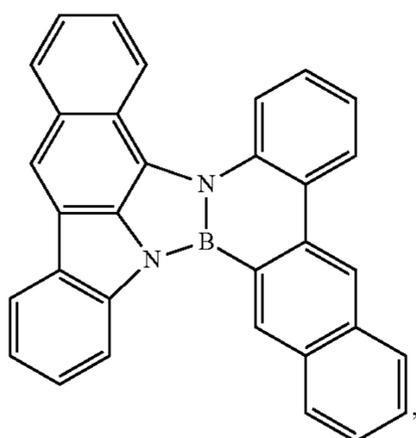
30

Compound 182



40

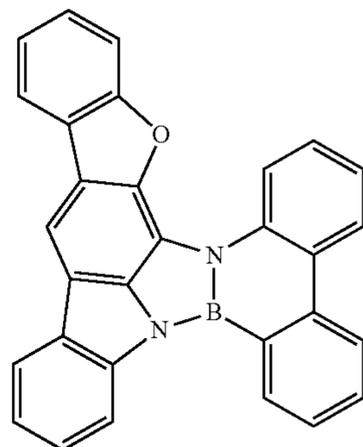
Compound 183



212

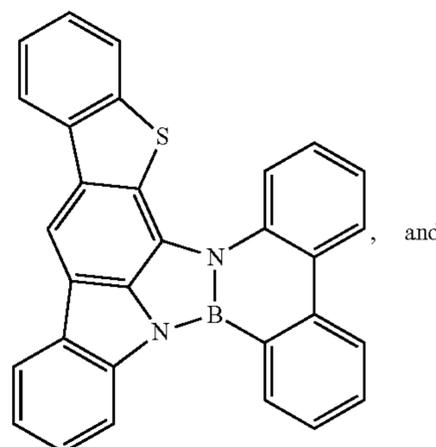
-continued

Compound 184



15

Compound 185

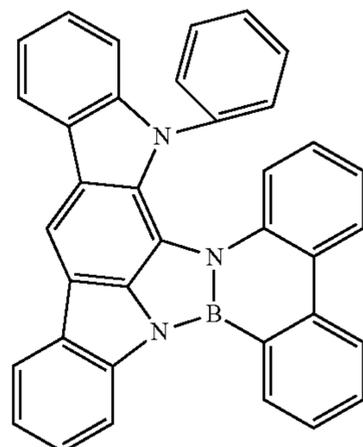


20

25

30

Compound 186



35

40

7. The compound of claim 1, wherein  $R^A$  is an aryl ring.8. The compound of claim 1, wherein  $R^B$  is an aryl ring or a heteroaryl ring comprising one hetero-atom selected from the group consisting of N, O, and S.9. The compound of claim 1, wherein  $R^C$  is an aryl ring or a heteroaryl ring comprising one or two nitrogen atoms.

10. The compound of claim 1, wherein:

- (a) at least one  $R^1$ ,  $R^2$ , or  $R^3$  comprises a substituent selected from the group consisting of carbazole, azacarbazole, dibenzofuran, azadibenzofuran, dibenzothiophene, azadibenzothiophene, dibenzoselenophene, azadibenzoselenophene, triphenylene, azatriphenylene, diphenyl(silyl), triphenyl(silyl), and tetraphenyl(silyl);
- (b) two adjacent substituents of  $R^1$ ,  $R^2$ , or  $R^3$  form a fused benzo substituent on  $R^A$ ,  $R^B$ , or  $R^C$ , respectively; or
- (c) both option (a) and option (b) are true.

11. The compound of claim 1, wherein at least one  $R^1$ ,  $R^2$ , or  $R^3$  comprises a substituent selected from the group consisting of carbazole, azacarbazole, dibenzofuran, azadibenzofuran, dibenzothiophene, azadibenzothiophene, dibenzoselenophene, azadibenzoselenophene, triphenylene, azatriphenylene, diphenyl(silyl), triphenyl(silyl), and tetraphenyl(silyl); and

the remaining substituents  $R^1$ ,  $R^2$ , and  $R^3$  are H.

213

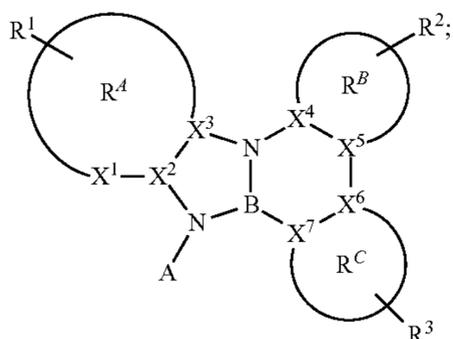
12. The compound of claim 1, wherein  $X^1$ - $X^6$  are C, and  $X^7$  is C or N.

13. A first organic light-emitting device comprising:

an anode;

a cathode; and

an organic layer, disposed between the anode and the cathode, comprising a compound having a structure of Formula I:



Formula I

wherein  $R^A$ ,  $R^B$ , and  $R^C$  are each independently 5 or 6 membered aryl or heteroaryl rings;

wherein  $R^1$ ,  $R^2$ , and  $R^3$  each independently represent no substitutions or up to the maximum available substitutions;

wherein  $R^1$ ,  $R^2$ , and  $R^3$  are each independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphine, a substituent of Formula I, and combinations thereof;

wherein any adjacent  $R^1$ ,  $R^2$ , and  $R^3$  are optionally joined or fused to form a ring;

wherein A is selected from the group consisting of halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphine, a substituent of Formula I, partially or fully deuterated variations thereof, and combinations thereof;

wherein A is optionally bonded to at least one benzo or azabenz ring to form fused rings;

wherein  $X^1$  is B, C, N, O, S or Se; and

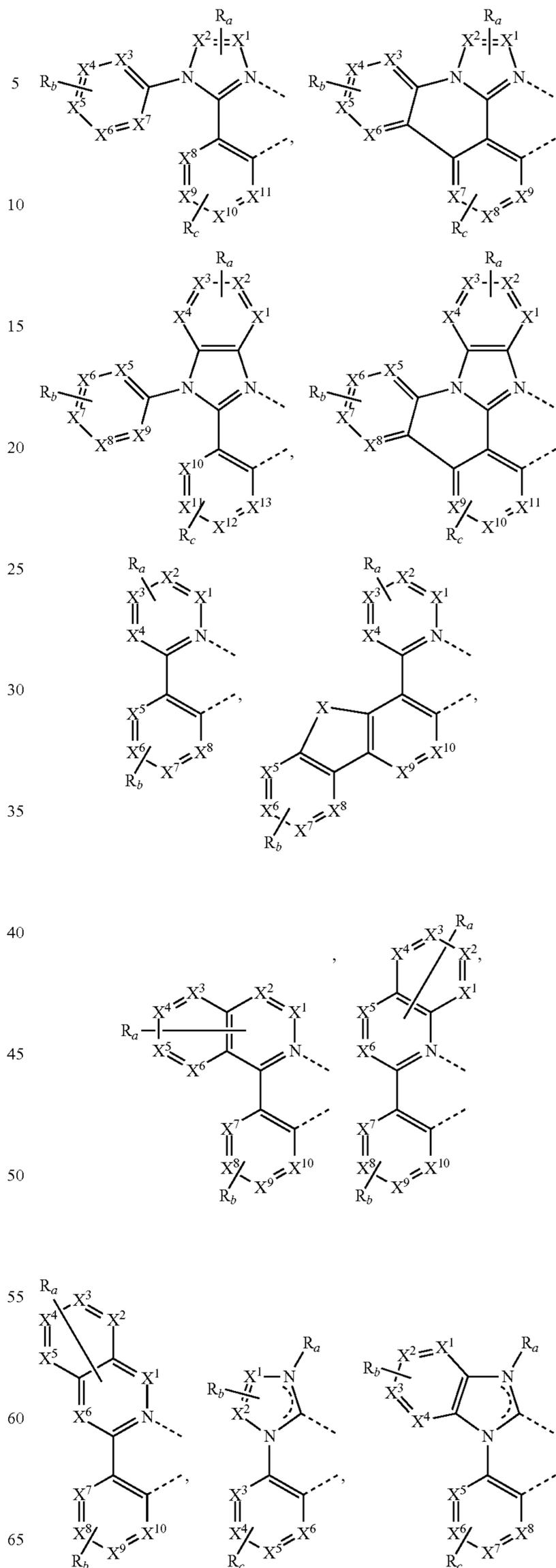
wherein  $X^2$ - $X^7$  are independently B, C or N.

14. The first device of claim 13, wherein the organic layer is an emissive layer and the compound is a host.

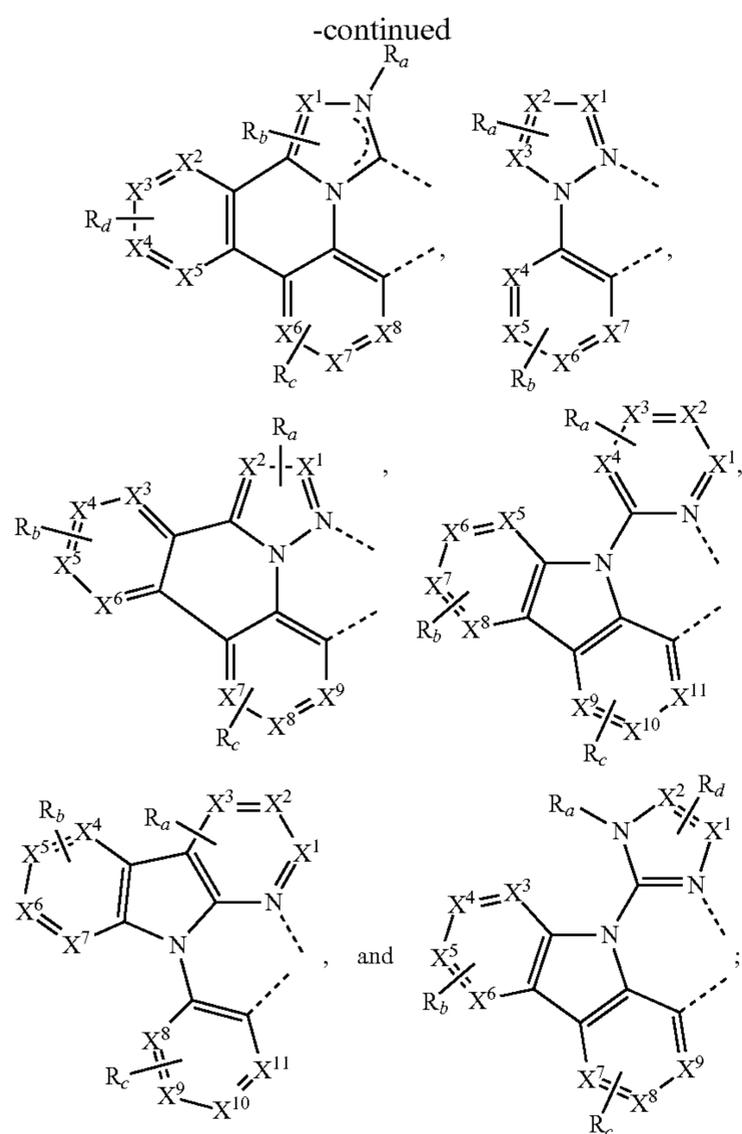
15. The first device of claim 13, wherein the organic layer further comprises an emissive dopant.

16. The first device of claim 15, wherein the emissive dopant is a transition metal complex having at least one ligand or part of the ligand, if the ligand is more than bidentate, selected from the group consisting of:

214



215



wherein each  $X^1$  to  $X^{13}$  are independently selected from the group consisting of carbon and nitrogen;

wherein X is selected from the group consisting of  $BR'$ ,  $NR'$ ,  $PR'$ , O, S, Se,  $C=O$ ,  $S=O$ ,  $SO_2$ ,  $CR'R''$ ,  $SiR'R''$ , and  $GeR'R''$ ;

wherein  $R'$  and  $R''$  are optionally fused or joined to form a ring;

wherein each  $R_a$ ,  $R_b$ ,  $R_c$ , and  $R_d$  may represent from mono substitution to the possible maximum number of substitutions, or no substitution;

wherein  $R'$ ,  $R''$ ,  $R_a$ ,  $R_b$ ,  $R_c$ , and  $R_d$  are each independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof; and

wherein any two adjacent substituents of  $R_a$ ,  $R_b$ ,  $R_c$ , and  $R_d$  are optionally fused or joined to form a ring or form a multidentate ligand.

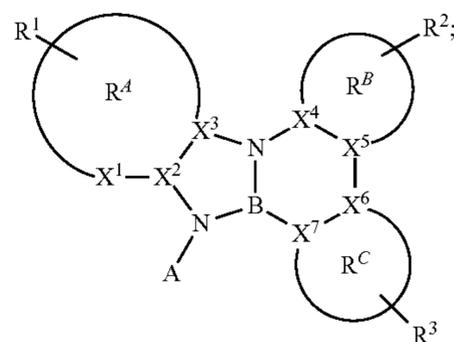
17. The first device of claim 13, wherein (i) the organic layer is a charge carrier blocking layer and the compound is a charge carrier blocking material in the organic layer, or (ii)

216

the organic layer is a charge carrier transporting layer and the compound is a charge carrier transporting material in the organic layer.

18. The first device of claim 13, wherein the first device is incorporated into a device selected from the group consisting of a consumer product, an electronic component module, an organic light-emitting device, and a lighting panel.

19. A formulation comprising a compound and one or more components selected from the group consisting of a solvent, a host, a hole injection material, hole transport material, and an electron transport layer material, wherein the compound has a structure of Formula I:



wherein  $R^A$ ,  $R^B$ , and  $R^C$  are each independently 5 or 6 membered aryl or heteroaryl rings;

wherein  $R^1$ ,  $R^2$ , and  $R^3$  each independently represent no substitutions or up to the maximum available substitutions;

wherein  $R^1$ ,  $R^2$ , and  $R^3$  are each independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphine, a substituent of Formula I, and combinations thereof;

wherein any adjacent  $R^1$ ,  $R^2$ , and  $R^3$  are optionally joined or fused to form a ring;

wherein A is selected from the group consisting of halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphine, a substituent of Formula I, partially or fully deuterated variations thereof, and combinations thereof;

wherein A is optionally bonded to at least one benzo or azabenzene ring to form fused rings;

wherein  $X^1$  is B, C, N, O, S or Se; and

wherein  $X^2$ - $X^7$  are independently B, C or N.

20. The compound of claim 1, A is not connected to  $X^1$  to form a fused ring.

\* \* \* \* \*